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Research Article

Modified Lennard-Jones Potentials with a Reduced Temperature-Correction Parameter for Calculating Thermodynamic and Transport Properties: Noble Gases and Their Mixtures (He, Ne, Ar, Kr, and Xe)

Seung-Kyo Oh

Pharmaceutics and Biotechnology Department, Konyang University, 121 University Road, Nonsan, Chungnam 320-711, Republic of Korea

Correspondence should be addressed to Seung-Kyo Oh; sunkist@konyang.ac.kr

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The three-parameter Lennard-Jones (12-6) potential function is proposed to calculate thermodynamic property (second virial coefficient) and transport properties (viscosity, thermal conductivity, and diffusion coefficient) of noble gases (He, Ne, Ar, Kr, and Xe) and their mixtures at low density. Empirical modification is made by introducing a reduced temperature-correction parameter τ to the Lennard-Jones potential function for this purpose. Potential parameters (σ, ε, and τ) are determined individually for each species when the second virial coefficient and viscosity data are fitted together within the experimental uncertainties. Calculated thermodynamic and transport properties are compared with experimental data by using a single set of parameters. The present study yields parameter sets that have more physical significance than those of second virial coefficient methods and is more discriminative than the existing transport property methods in most cases of pure gases and of gas mixtures. In particular, the proposed model is proved with better results than those of the two-parameter Lennard-Jones (12-6) potential, Kihara Potential with group contribution concepts, and other existing methods.

1. Introduction

Accurate representation of thermodynamic and transport properties is essential to process engineers to design and optimize equipment and chemical processes. Second virial coefficient is an important quantity which is useful in calculating vessel size from volumetric data, heating requirements from calorimetric data, and stage requirements from phase equilibrium data. Transport properties such as viscosity, thermal conductivity, and diffusion coefficient are critically important parameters in many engineering applications: for the determination of pipeline, heatexchanger and separation equipment size, mass transfer efficiency of reservoir of oils, and the power required to pump fluid [1].

The intermolecular forces are of great importance to scientists in a wide field of disciplines as information of these interactions provides the progress of collisions between molecules and determines the bulk properties of substances. Approximation of thermodynamic and transport properties from statistical mechanics requires a realistic intermolecular potential [2]. The theoretical basis in statistical mechanics for the virial equation is one of its attractions. The viral equation truncated after the second term is a popular tool to calculate accurate thermodynamic properties at low or moderate densities. A number of investigators have emphasized the determination of second virial coefficient through experiments and correlations. When Chapman-Enskog gas kinetic theory [3] allows the prediction of transport properties, the potential energy of molecular interactions is known as a function of intermolecular separation and orientation. A description of the spherically symmetric potential as a function of intermolecular separation, averaged over all molecular orientations, suffices to calculate dilute gas viscosities, thermal conductivities, and diffusion coefficients of monoatomic gases.

A realistic intermolecular potential allows the calculation of thermodynamic and transport properties. A lot of studies have focused on individual properties like second virial coefficient or viscosity for the determination of intermolecular potential parameters [2]. Potential parameters of any given model that give the best fit for thermodynamic and transport properties (e.g., second virial coefficient, viscosity, thermal conductivity, and diffusion coefficient) are generally different. Therefore, for a simple model such as Lennard-Jones potential, there is one specific set of potential parameters suitable for each property, producing significantly different results [4].

Several investigators [2, 5–7] have used statistical mechanics and kinetic theory of gases to represent thermodynamic and transport properties with a single set of molecular parameters, namely, those appearing in an intermolecular potential function. The Lennard-Jones (12-6) potential has been widely used for the representation of thermodynamic and transport properties of normal fluids. In one particularly interesting study of Tee et al. [6], a single set of molecular parameters was evaluated from the Lennard-Jones (12-6) potential for each species; in this procedure, viscosity data for each substance was fitted first by least-squares analysis, second virial coefficient was fitted next, and the data on second virial coefficient and viscosity were statistically analyzed simultaneously to develop corresponding states correlations with a single set of potential parameters for each substance. They concluded that when second virial coefficient and viscosity data were fitted together, their sets of molecular parameters give the best overall fit to the data for each species and tend to be least affected by experimental errors; beside that their results are quite comparable to those determined individually from viscosity. Potential parameters obtained in this manner were proved to be successful in predicting second virial coefficients and dilute gas viscosities for molecules ranging in shape from spherical to chains as long as n-heptane with good result. Hence, the Lennard-Jones potential is still attractive for its simplicity and capability of predicting noble gas properties if its weak point is compensated for and its accuracy is improved.

The objective of this study is to represent thermodynamic property (second virial coefficient) and transport properties (viscosity, thermal conductivity, and diffusion coefficient) of noble gases (He, Ne, Ar, Kr, and Xe) and their binary mixtures at low density using a single set of modified Lennard-Jones (12-6) potential parameters. For this purpose, a temperature-correction parameter was introduced to the reduced temperature T^* in the Lennard-Jones (12-6) potential function. A set of potential parameters was determined when the second virial coefficient and viscosity data are fitted simultaneously within their experimental errors, separately for each noble gas; parameters obtained in this manner were used in all subsequent calculations of properties such as thermal conductivity and diffusion coefficient, in which data were not supplied to parameter estimations, and in mixture property computations. Validity of the modified Lennard-Jones (12-6) potential with a reduced temperature-correction parameter was tested with good results in comparison with other existing methods.

2. Theory

In this paper, special focus was placed on the Lennard-Jones (12-6) intermolecular potential for the computations of noble gas properties, even though more accurate potentials exist. A form of this potential was first established by Lennard-Jones [8] and is a mathematically simple model that approximates the interaction between a pair of neutral atoms or molecules. The most common expression of the Lennard-Jones (12-6) potential has the form

$$U(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \tag{1}$$

where $U(r)$ is the intermolecular potential energy as a function of the separation distance between a pair of molecules, ε is the depth of the potential well in Joule, and σ is the finite distance in angstrom Å at which the interparticle potential becomes zero.

These potential parameters can be fitted by least-squares analysis and lead to provide accurate calculations of dilute gas thermodynamic property (second virial coefficient) and transport properties (viscosity, thermal conductivity, and diffusion coefficient) of noble gases, as summarized below.

2.1. Second Virial Coefficient.

2.1. Second Virial Coefficient. From statistical mechanics, the relations between second virial coefficient and intermolecular potential functions were theoretically derived; in particular, explicit expression of the second virial coefficient for the Lennard-Jones (12-6) potential was rigorously derived by Hirschfelder et al. [4] for a computational use:

$$B(T) = -\frac{2}{3}\pi N_A \sigma^3 \sum_{n=0}^{\infty} \frac{2^{n+1/2}}{4n!} \Gamma\left(\frac{2n-1}{4}\right) T^{*-(2n+1)/4} \tag{2}$$

in which N_A is the Avogadro's constant $6.022\cdot10^{23}$ mol^{-1}, T^* is the reduced (dimensionless) temperature $k_B T/\varepsilon$, and κ_B is the Boltzmann constant $1.3806488\cdot10^{-23}$ JK^{-1}. However, Kojima [9] observed that it is quite effective for calculating virial coefficients from the Stockmayer intermolecular potential model with an aid of introducing a reduced temperature-correction parameter of τ as $(T - \tau)$ instead of using temperature T. This temperature-correction parameter was also proved in developing a new virial equation of state by Ichikura et al. [10].

In the present study, our observations on the accurate approximation not only of thermodynamic property (second virial coefficient), but also of transport properties (viscosities, thermal conductivities, and diffusion coefficients) in the dilute gaseous phase of noble gases were made by introducing temperature-correction parameter τ to the reduced temperature T^* shown in the Lennard-Jones (12-6) potential function:

$$T^* = \frac{\kappa_B (T - \tau)}{\varepsilon}. \tag{3}$$

Then the second virial coefficient can be calculated from (2) and (3) when three potential parameters (σ, ε, and τ) of the modified Lennard-Jones (12-6) potential are fitted together to second virial coefficient and viscosity data separately for each substance.

For interaction of different molecular species, the combining rules are used for the molecular distance, energy, and reduced temperature-correction parameter for mixture computations:

$$\sigma_{12} = \frac{\sigma_1 + \sigma_2}{2}, \tag{4}$$

$$\varepsilon_{12} = \left(\varepsilon_1 \varepsilon_2\right)^{1/2}, \tag{5}$$

$$\tau_{12} = \frac{\tau_1 + \tau_2}{2}. \tag{6}$$

For spherical molecules, these equations are of high accuracy for the prediction of second cross-virial coefficient B_{12} required in (2) and other mixture properties discussed later.

2.2. Viscosity. Transport properties (viscosity, thermal conductivity, and diffusion coefficient) at low density can be calculated by using Chapman-Enskog kinetic theory [3], which has been applied rigorously to monatomic gases in a number of studies [11]. The dilute gas viscosity can be well presented by the Chapman-Enskog approximation derived from the kinetic theory:

$$\eta = 26.693 \frac{\sqrt{MT}}{\sigma^2 \Omega^{(2,2)^*}\left(T^*\right)}, \tag{7}$$

where M is the molecular weight (gram mol^{-1}), T is the absolute temperature in Kelvin, and the viscosity η is in micropoise μP. For mixture viscosity calculations, the formula proposed by Hirschfelder et al. [4] was used in this study, in which the interaction quantity η_{12} must be determined to employ this method in advance:

$$\eta_{12} = 26.693 \frac{\sqrt{2M_1 M_2 T / \left(M_1 + M_2\right)}}{\sigma^2{}_{12} \Omega^{(2,2)^*}\left(T^*_{12}\right)} \tag{8}$$

in which M_1 and M_2 are the molecular weights of the components 1 and 2, respectively, and $T^*{}_{12}$ is the modified reduced temperature for mixture calculations, $k_B(T - \tau_{12})/\varepsilon_{12}$. The composition dependence of viscosity on the binary gas mixture is defined as follows:

$$\frac{1}{\eta_{\text{mix}}} = \frac{X_\eta + Y_\eta}{1 + Z_\eta}, \tag{9}$$

$$X_\eta = \frac{{y_1}^2}{\eta_1} + \frac{2 y_1 y_2}{\eta_{12}} + \frac{{y_2}^2}{\eta_2}, \tag{10}$$

$$\begin{aligned} Y_\eta = \frac{3}{5} A^*{}_{12} \left[\frac{{y_1}^2}{\eta_1}\left(\frac{M_1}{M_2}\right) + \frac{2 y_1 y_2}{\eta_{12}} \left[\frac{\left(M_1 + M_2\right)^2}{4 M_1 M_2}\right] \right. \\ \left. \times \left(\frac{{\eta_{12}}^2}{\eta_1 \eta_2}\right) + \frac{{y_2}^2}{\eta_2}\left(\frac{M_2}{M_1}\right) \right], \end{aligned} \tag{11}$$

$$\begin{aligned} Z_\eta = \frac{3}{5} A^*{}_{12} \left[{y_1}^2 \left(\frac{M_1}{M_2}\right) + 2 y_1 y_2 \right. \\ \times \left[\frac{\left(M_1 + M_2\right)^2}{4 M_1 M_2} \left(\frac{\eta_{12}}{\eta_1} + \frac{\eta_{12}}{\eta_2} - 1\right) \right] \\ \left. + {y_2}^2 \left(\frac{M_2}{M_1}\right) \right], \end{aligned} \tag{12}$$

$$A^*{}_{12} = \left(\frac{\Omega^{(2,2)^*}}{\Omega^{(1,1)^*}}\right), \tag{13}$$

where η_{mix} is the mixture viscosity, and y_i, M_i, and η_i are the mole fractions, the molecular weights, and the viscosities at the mixture temperature of the pure components i ($i = 1, 2$). And the quantities $\Omega^{(2,2)^*}$ and $\Omega^{(1,1)^*}$ are the collision integrals for viscosity and diffusion coefficient, respectively, and are defined as a function of the reduced temperature T^* which depends on the intermolecular potential selected. Neufeld et al. [12] proposed analytical approximations to transport collision integrals for the Lennard-Jones (12-6) potential in the range $0.3 < T^* < 100$, being convenient for easy computer application:

$$\begin{aligned} \Omega^{(2,2)^*}\left(T^*\right) = \frac{1.16145}{T^{*0.14874}} + \frac{0.52487}{\exp\left(0.77320 T^*\right)} \\ + \frac{2.16178}{\exp\left(2.43787 T^*\right)}, \end{aligned} \tag{14}$$

$$\begin{aligned} \Omega^{(1,1)^*}\left(T^*\right) = \frac{1.06036}{T^{*0.15610}} + \frac{0.1930}{\exp\left(0.47635 T^*\right)} \\ + \frac{1.03587}{\exp\left(1.52996 T^*\right)} + \frac{1.76474}{\exp\left(3.89411 T^*\right)}. \end{aligned} \tag{15}$$

2.3. Thermal Conductivity. Since the Chapman-Enskog gas kinetic theory uses a common basis for the evaluation of viscosity and thermal conductivity, the statistical expression for the thermal conductivity involves the same collision integral as does the viscosity. For a pure monoatomic gas at low density, which has no rotational or vibrational degrees of freedom, thermal conductivity was calculated through a rigorous analysis by Brokaw [13]:

$$\lambda = 0.0026693 \frac{\sqrt{T/M}}{\sigma^2 \Omega^{(2,2)^*}\left(T^*\right)} = \frac{15}{4}\left(\frac{R}{M}\right)\eta, \tag{16}$$

where the thermal conductivity λ is microwatts per meter per degree Kelvin in mW m^{-1} K^{-1} and R is the universal gas constant 83.14 cm^3 bar mol^{-1} k^{-1}. Thus, the thermal conductivity of the noble gas can be calculated from the estimated potential parameters or from experimental viscosity data which are generally available for the molecule. In the present work, pure viscosity value obtained from (7) was used for the calculation of thermal conductivity of pure substance. It thus implies that a check on the thermal conductivity serves as a cross-check between the viscosity and thermal conductivity

Table 1: Potential parameters of Lennard-Jones (12-6) Potential with a reduced temperature-correction parameter.

Group	σ/Å	(ε/κ_B)/K	τ/K
Helium	2.628	5.465	−0.836
Neon	2.775	36.831	−2.468
Argon	3.401	116.81	5.642
Krypton	3.601	164.56	11.41
Xenon	4.055	218.18	13.09

data and not necessarily as a check on the potential function chosen [14].

Various prediction methods for estimating mixture thermal conductivity have appeared, one of which is essentially empirical and it is reduced to some form of the Wassiljewa equation [15]:

$$\lambda_{\text{mix}} = \sum_{i=1}^{n} \frac{y_i \lambda_i}{\sum_{j=1}^{n} y_j A_{ij}}, \tag{17}$$

where λ_{mix} is the mixture thermal conductivity and A_{ij} is a combinational factor. This factor is empirically expressed by Mason and Saxena [16] as

$$A_{ij} = \frac{1.065}{2\sqrt{2}} \frac{\left[1 + \left(\lambda_i/\lambda_j\right)^{1/2} \left(M_i/M_j\right)^{1/4}\right]^2}{\left(1 + M_i/M_j\right)^{1/2}}, \tag{18}$$

where λ_i are the thermal conductivities of pure component determined from (16), which are sufficient to predict mixture thermal conductivity when its measurements are not available in the literature.

2.4. Diffusion Coefficient.

The Chapman-Enskog expression for binary diffusion coefficient of dilute gas is presented by Hirschfelder et al. [4]:

$$D_{12} = 0.0026693 T^{3/2} \frac{\sqrt{\left(M_1 + M_2\right)/2M_1 M_2}}{P{\sigma^2}_{12} \Omega^{(1,1)^*}\left({T^*}_{12}\right)}, \tag{19}$$

where D_{12} is in $\text{cm}^2\,\text{sec}^{-1}$ and P is in bar. And $\Omega^{(1,1)^*}$ is the collision integral for diffusion coefficient of nonpolar Lennard-Jones (12-6) potential given by (15). When molecules 1 and 2 are identical, (19) becomes expression for the self-diffusion coefficient:

$$D = 0.0026693 T^{3/2} \frac{\sqrt{1/M}}{P\sigma^2 \Omega^{(1,1)^*}\left(T^*\right)}. \tag{20}$$

3. Results and Discussion

3.1. Pure Noble Gases.

As a part of systematic program of our researches, modified Lennard-Jones (12-6) potential function with a reduced temperature-correction parameter was applied to noble gases (He, Ne, Ar, Kr, and Xe) for the computation of thermodynamic (second virial coefficient) and transport properties (viscosity, thermal conductivity, and self-diffusion coefficient) at low density.

Using (2), (3), and (7), three potential parameters (σ, ε, and τ) were evaluated from the simultaneous regression of second virial coefficient and viscosity data separately for each species. For instance, three parameter values ($\sigma_{\text{He}}, \varepsilon_{\text{He}}$, and τ_{He}) for helium gas were determined from second virial coefficient and viscosity data of pure helium gas. Potential parameters of other noble gases were evaluated in an analogous manner.

A critical review of the literature on second virial coefficient was achieved by Dymond et al. [17]. They provided the recommended values of virial coefficients for each compound fitted to a smoothing function of temperature by the least-squares criterion. This smoothing function for second virial coefficient is the polynomial of reciprocal temperature with usually three terms. In particular, two different smoothing correlations of helium were given in the temperature ranges between 1.59 K and 35.1 K and between 35.1 K and 1473.15 K. We have used their comprehensive compilation of the second virial coefficient data as our data source. And pure viscosity data required for the potential parameter determinations were all taken from Stephan and Lucas [18], even though other recommended or various sets of data exist. Nonlinear least-squares parameter estimation subroutine based on the Levenberg-Marquardt algorithm supplied by IMSL STAT/library [19] was used in this data regression, in which each data point was weighted by its estimated experimental uncertainty taken from the corresponding Refs. A set of potential parameters individually for each substance can then be estimated when the following objective function is minimized:

$$\Phi = \sum_{i=1}^{n_B} \left(\frac{B_{i,\text{obsd}} - B_{i,\text{calc}}}{\delta_{i,B}}\right)^2 + \sum_{i=1}^{n_\eta} \left(\frac{\eta_{i,\text{obsd}} - \eta_{i,\text{calc}}}{\eta_{i,\text{obsd}}\delta_{i,\eta}}\right)^2 \tag{21}$$

in which δ_B is the observed uncertainty of second virial coefficient in $\text{cm}^3\,\text{mol}^{-1}$ and δ_η is of dimensionless fractional uncertainty of viscosity in %. It is noted that the first term is designated for second virial coefficient and the second for viscosity.

Table 1 summarizes determined parameter values of modified Lennard-Jones (12-6) potential (σ, ε, and τ) of noble gases (He, Ne, Ar, Kr, and Xe). In Table 2, resulting deviations between observed and regressed second virial coefficient data are given on an RMSD (root-mean-square deviation) basis in $\text{cm}^3\,\text{mol}^{-1}$, which is defined by

$$\text{RMSD} = \sqrt{\frac{1}{n_B} \sum_{i=1}^{n_B} \left(B_{i,\text{obsd}} - B_{i,\text{calc}}\right)^2}. \tag{22}$$

Comparisons of the proposed method with other existing methods are shown in Table 2 along with their data sources and observed temperature ranges. The average RMSD between a total of observed and calculated 735 second virial coefficient data of five noble gases by the present method was $3.33\,\text{cm}^3\,\text{mol}^{-1}$, indicating that the proposed method compares very well with the Dymond's correlations

Table 2: Deviations between experimental and calculated second virial coefficients of pure noble gases.

Compound	Number of data points	Average RMSD in B ($\mathrm{cm^3\,mol^{-1}}$)						
		Present study	Dymond et al.	L-J	Kihara	Tsonopoulos	ΔT (K)	Reference
Regression results								
Helium	304	5.44	5.07[a]	10.9	10.8	39.1	2–1473	[2]
Neon	55	0.28	0.34	0.45	1.38	1.56	44–873	[2]
Argon	105	0.40	0.53	2.43	1.73	1.88	75–773	[2]
Krypton	157	2.87	3.18	5.75	3.67	6.90	107–873	[2]
Xenon	114	2.50	2.67	4.32	2.53	3.51	160–973	[2]
Average	735	3.33	3.29	6.79	5.99	18.6		
Prediction results								
Helium	8	4.13	1.08	10.8	4.29	14.9	343–374	[27]
Xenon	9	0.50	1.37	2.57	2.11	2.57	206–273	[28]
Average	17	2.21	1.23	6.44	3.14	8.37		

[a] Two different smoothing functions were used in the temperature ranges between 1.59 K and 35.1 K, and between 35.1 K and 1473.15 K.

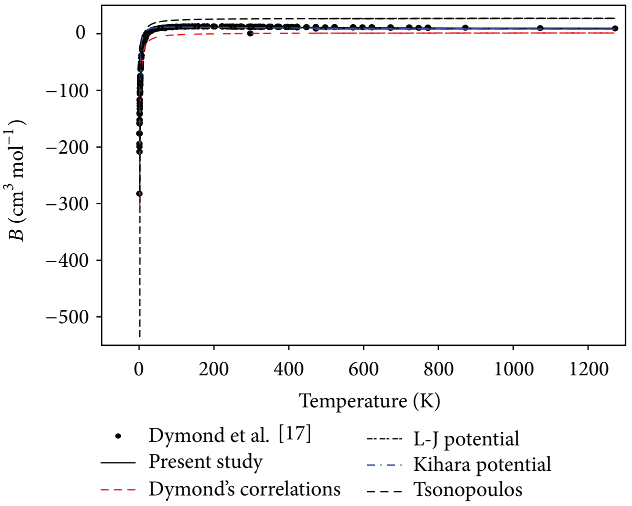

Figure 1: Comparison of measured and calculated second virial coefficients for He.

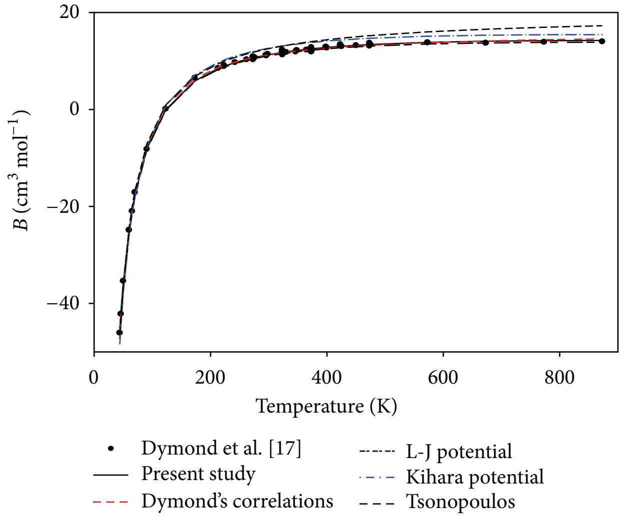

Figure 2: Comparison of measured and calculated second virial coefficients for Ne.

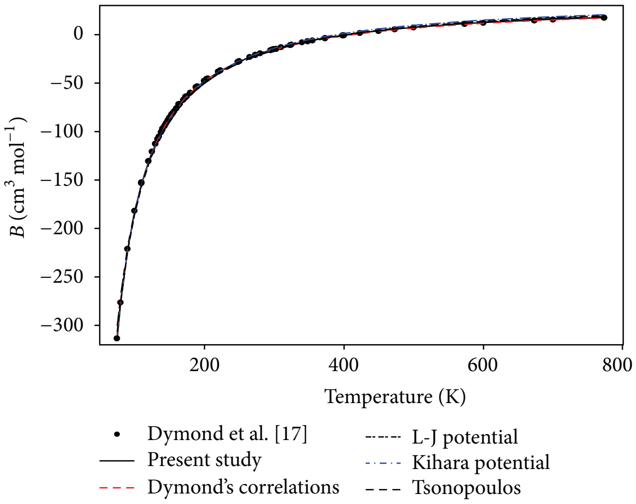

Figure 3: Comparison of measured and calculated second virial coefficients for Ar.

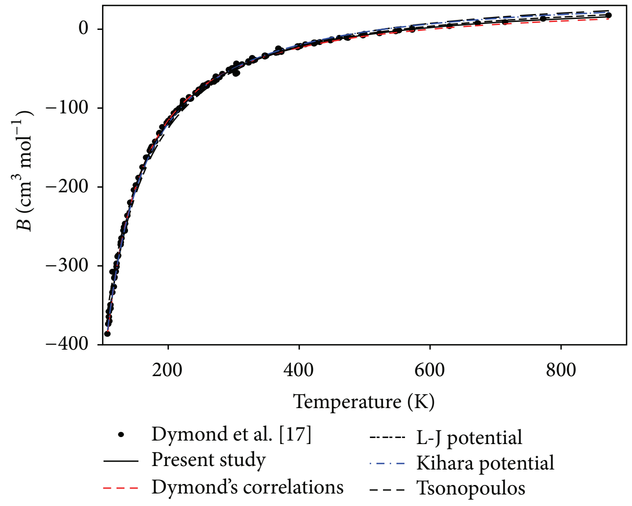

Figure 4: Comparison of measured and calculated second virial coefficients for Kr.

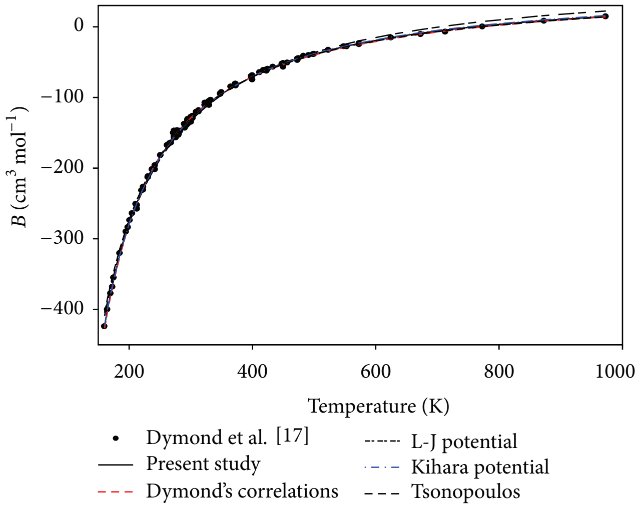

FIGURE 5: Comparison of measured and calculated second virial coefficients for Xe.

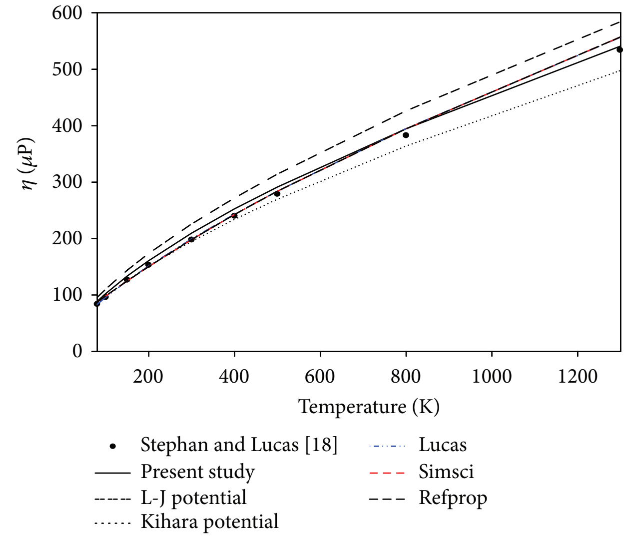

FIGURE 6: Comparison of measured and calculated viscosities for He.

[17] 3.29 cm^3 mol^{-1} and yields more accurate results than other existing methods: original two-parameter Lennard-Jones (12-6) potential [4] 6.79 cm^3 mol^{-1}, Kihara potential with group contribution concept [20] 5.99 cm^3 mol^{-1}, and the corresponding states method of Tsonopoulos [21] 18.6 cm^3 mol^{-1}. A comparison of the measured and calculated second virial coefficients from Dymond et al. [17] for pure noble gases (He, Ne, Ar, Kr, and Xe) is presented in Figures 1, 2, 3, 4, and 5, in order. Also included in Table 2 are prediction results from other second virial coefficient data of helium and xenon available in the literature, showing similar results.

In Table 3, deviations of regression results between observed and calculated viscosity data are presented on an RMSD$_\mathrm{r}$

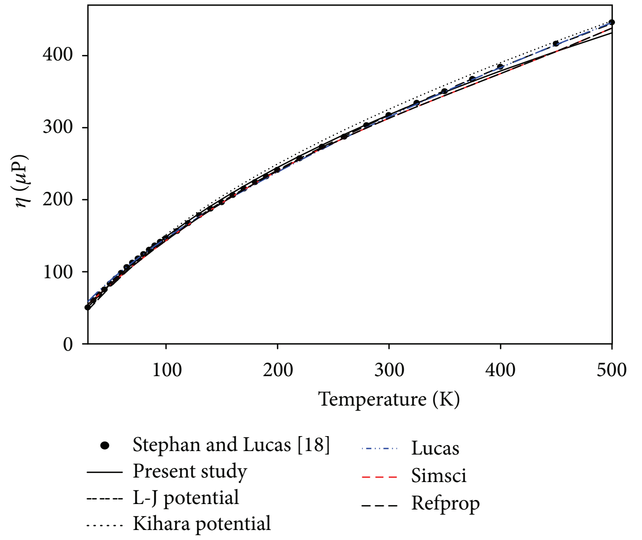

FIGURE 7: Comparison of measured and calculated viscosities for Ne.

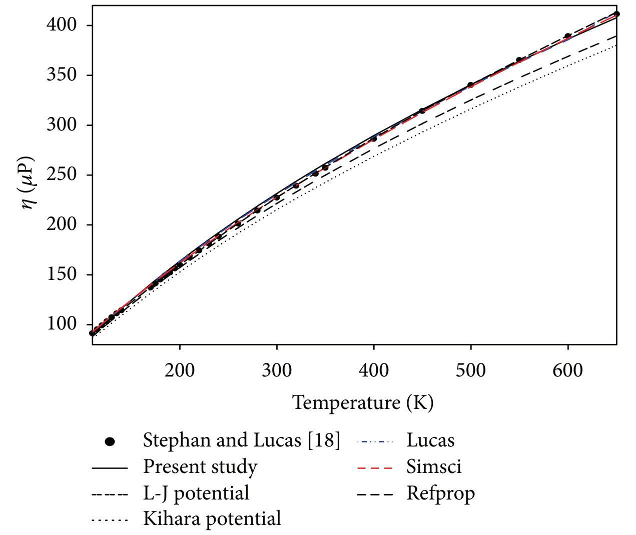

FIGURE 8: Comparison of measured and calculated viscosities for Ar.

(root-mean-square deviation, relative) basis in %, which is defined by

$$\mathrm{RMSD_r} = \sqrt{\frac{1}{n_\eta}\sum_{i=1}^{n_\eta}\left(\frac{\left(\eta_{i,\mathrm{obsd}} - \eta_{i,\mathrm{calc}}\right)}{\eta_{i,\mathrm{obsd}}}\right)^2}. \qquad (23)$$

The average RMSD$_\mathrm{r}$ value between a total of observed and regressed 117 viscosity data for five noble gases was found to be 1.90%, indicating that the present work is quite comparable to the Refprop Database correlations [22] 1.78% and is in better agreement with experimental data than any other existing methods: original Lennard-Jones (12-6) potential 6.60%, Kihara potential with group contribution concept 5.74%, the corresponding states method of Lucas [23] 2.25%, and the Simsci Database correlations [24] 2.08%.

Table 3: Deviations between experimental and calculated viscosities of pure noble gases.

Compound	Number of data points	Average RMSD$_r$ in η (%)							
		Present study	L-J	Kihara	Lucas	Simsci	Refprop	ΔT (K)	Reference
		Regression results							
Helium	9	5.27	18.3	13.2	3.23	2.05	2.83	80–1300	[24]
Neon	36	1.50	1.86	3.76	2.80	4.29	2.48	30–500	[24]
Argon	30	1.84	2.72	5.33	1.73	1.32	0.29	10–650	[24]
Krypton	19	2.87	12.2	8.56	1.23	0.91	1.85	150–600	[24]
Xenon	23	0.49	9.88	4.10	2.50	0.57	2.13	300–430	[24]
Average	117**	1.90	6.60	5.74	2.25	2.08	1.78		
		Prediction results							
Helium	22	4.11	8.33	2.99	4.95	0.98	3.94	50–973	[26]
	31	4.62	9.03	2.96	3.92	0.60	10.0	20–1000	[29]
	1	4.44	8.82	0.76	2.87	0.64	1.32	300	[30]
	8	2.34	6.52	4.03	6.74	0.91	0.84	298–1010	[31]
	1	4.83	9.93	0.14	2.26	0.06	0.75	303	[32]
	13	3.15	7.32	4.24	6.36	1.31	1.43	198–473	[33]
	8	2.90	6.86	4.17	6.42	0.40	0.53	298–973	[34]
	8	2.71	6.65	4.27	6.54	0.23	0.42	298–973	[35]
	6	2.98	6.87	4.37	6.55	0.36	0.57	298–973	[36]
	9	3.26	7.90	2.47	4.72	0.33	0.49	298–678	[37]
	9	2.51	6.68	3.83	6.17	0.26	0.36	298–778	[38]
	5	4.05	8.85	1.32	3.48	0.09	0.41	298–473	[39]
	1	2.91	7.66	2.66	5.3	3.68	3.46	767	[40–42]
	6	4.24	8.91	1.37	3.54	0.35	0.32	298–512	[43]
	1	5.28	10.2	0.08	2.03	0.09	0.62	292	[44]
	1	5.72	10.5	0.77	1.34	0.76	0.03	291	[45, 46]
	2	6.29	11.1	1.40	0.98	1.39	0.76	291	[47]
	2	5.06	10.1	12.7	2.12	0.13	0.60	293–303	[48]
	4	5.48	10.4	0.95	1.82	0.51	0.81	237–308	[49]
	6	5.91	10.7	1.51	0.36	1.50	2.50	72–291	[50]
	10	5.01	9.61	4.31	1.77	3.08	30.8	14–293	[51]
	5	5.30	10.2	0.46	2.23	1.84	1.83	297–523	[52]
	2	5.07	10.1	0.13	2.11	0.12	0.59	293–303	[53]
	1	4.85	9.99	0.02	2.16	0.14	0.54	303	[54]
	10	4.94	9.75	1.01	2.86	1.40	1.38	293–523	[55]
	39	6.84	10.4	2.73	6.18	5.94	22.0	14–973	[56]
	74	3.40	7.42	3.73	5.97	0.87	0.58	100–1000	[57]
	72	5.77	10.3	6.75	4.09	15.7	62.2	200–1000	[58]
	8	2.69	6.63	4.28	6.55	0.24	0.44	298–973	[59]
	11	4.70	9.22	1.89	3.51	0.46	0.49	100–600	[60]
	19	5.32	9.72	3.05	4.30	0.35	1.68	80–1000	[61]
	7	1.32	4.25	5.50	7.98	3.10	3.45	250–1000	[62]
	13	3.83	8.54	1.89	4.34	2.64	2.53	373–973	[63]
Average	415*	4.49	8.76	3.75	4.82	3.97	15.1		
Neon	27	2.04	1.54	8.00	3.14	3.04	15.2	50–973	[26]
	6	1.58	1.22	7.79	2.45	1.47	2.20	100–600	[29]
	8	1.58	0.72	8.36	3.65	0.57	27.4	298–973	[64]
	13	1.83	1.04	8.60	3.54	1.04	21.2	298–973	[33]
	8	2.07	1.24	8.91	4.21	0.92	27.1	298–973	[35]
	6	2.22	1.37	8.97	4.30	1.09	29.8	298–973	[36]

Table 3: Continued.

Compound	Number of data points	Average RMSD$_r$ in η (%)							
		Present study	L-J	Kihara	Lucas	Simsci	Refprop	ΔT (K)	Reference
	8	2.27	1.39	9.05	4.36	1.08	26.9	298–973	[65]
	5	1.13	0.46	7.91	1.82	1.07	2.72	298–473	[39]
	7	1.80	1.00	8.66	3.64	0.91	11.3	298–778	[38]
	9	1.67	0.90	8.47	2.90	1.15	3.52	298–673	[37]
	3	1.07	2.10	5.89	0.82	0.66	0.47	298–348	[66]
	3	4.46	5.53	2.74	4.21	3.99	2.91	298–348	[67, 68]
	3	0.49	1.50	6.45	0.29	0.13	1.07	298–348	[69]
	6	1.03	2.01	6.02	0.81	0.70	0.71	298–348	[40–42]
	3	0.27	1.17	6.78	0.22	0.58	1.39	298–348	[70]
	3	0.19	1.17	6.76	0.22	0.33	1.39	298–348	[71]
	3	0.75	0.75	7.36	0.97	1.00	2.11	298–348	[72]
	3	0.56	0.52	7.38	0.81	0.97	2.04	298–348	[73]
	3	0.49	0.56	7.32	0.74	0.92	1.98	298–348	[74]
	3	1.09	0.89	7.56	1.30	1.28	2.38	298–348	[75]
	3	0.58	0.50	7.39	0.83	0.99	2.06	298–348	[76]
	4	0.65	0.305	7.45	0.64	1.61	1.71	237–308	[49]
	2	0.65	0.328	7.50	0.78	1.35	1.94	293–303	[53]
	5	2.20	1.986	8.31	2.24	2.10	3.38	72–291	[77]
	5	1.08	2.994	8.15	1.92	9.59	7.60	20–293	[51]
	6	2.08	2.176	7.54	2.44	2.05	2.91	273–523	[52]
	2	0.65	0.328	7.50	0.78	1.35	1.94	293–303	[53]
	2	1.12	2.129	5.76	1.14	0.47	0.17	291	[47]
	2	0.52	0.947	6.98	0.51	0.92	1.39	291	[45, 46]
	52	0.98	1.568	7.83	1.68	6.64	13.4	20–1000	[56]
	32	1.24	0.991	7.71	3.11	0.68	22.1	100–950	[57]
	92	4.80	4.116	5.86	4.23	12.4	7.89	27–320	[58]
	8	2.08	1.242	8.92	4.21	0.93	27.1	298–973	[59]
	11	1.77	2.693	5.38	1.53	1.83	1.92	100–600	[60]
	19	1.35	1.439	7.15	2.68	1.10	20.4	80–1000	[61]
	1	1.28	2.29	5.60	1.30	0.60	0.14	291	[48]
	4	1.04	2.09	5.92	0.57	1.51	0.71	293–523	[78]
Average	380*	2.25	2.07	7.24	2.87	4.83	12.0		
Argon	22	2.37	2.77	7.56	2.17	2.23	2.14	50–973	[26]
	63	2.78	2.25	5.85	2.38	2.98	1.94	90–500	[79]
	28	1.63	1.99	6.96	1.73	1.48	1.06	87–1000	[29]
	19	2.45	2.04	6.46	2.02	1.55	8.98	173–1597	[80]
	1	1.71	0.48	6.00	0.18	0.17	0.02	298	[32]
	8	1.14	2.59	8.39	2.39	0.58	1.47	298–973	[64]
	11	0.88	2.64	8.05	1.96	0.87	0.90	298–473	[33]
	6	1.20	2.92	8.25	2.23	0.97	0.61	298–767	[81]
	9	1.48	3.43	8.85	2.86	1.20	3.30	298–1124	[31]
	8	1.17	3.03	8.45	2.43	0.63	1.54	298–973	[35]
	7	1.21	2.97	8.24	2.36	0.73	1.41	298–973	[65]
	5	0.92	1.99	7.36	1.33	0.95	0.62	298–473	[82]
	5	0.85	1.95	7.36	1.29	0.92	0.60	300–473	[83]
	2	8.16	6.93	11.4	5.32	6.43	7.39	55–90	[84]
	1	2.01	0.12	5.79	0.34	0.31	0.07	273	[85]
	1	3.90	1.56	4.81	1.25	6.76	26.7	1373	[86]
	1	1.98	0.21	5.77	0.41	0.40	0.19	293	[87]
	1	2.99	0.62	5.40	0.89	5.27	12.3	1100	[40–42]

Table 3: Continued.

Compound	Number of data points	Average RMSD$_r$ in η (%)							
		Present study	L-J	Kihara	Lucas	Simsci	Refprop	ΔT (K)	Reference
	1	5.90	3.55	3.33	2.25	9.28	80.4	1873	[88]
	9	0.94	2.79	8.22	2.08	0.80	0.49	298–773	[38]
	6	1.18	2.84	8.17	2.16	0.85	0.45	298–770	[89]
	8	0.93	2.68	8.07	1.95	0.93	0.46	298–673	[37]
	21	2.21	0.83	5.73	0.83	0.89	0.39	202–394	[90]
	5	12.8	13.9	17.4	13.6	12.2	11.4	775–1053	[40–42]
	7	12.0	12.7	15.9	12.5	11.7	29.9	775–1838	[76]
	5	3.75	1.70	5.30	1.20	5.79	36.5	569–1838	[91]
	6	5.64	4.66	8.52	3.63	3.25	3.96	72–291	[50]
	2	1.79	0.44	11.2	0.27	0.26	0.11	293–303	[48]
	1	2.19	0.01	5.59	0.60	0.58	0.37	291	[45, 46]
	5	5.22	4.39	8.44	3.36	3.00	3.72	72–291	[77]
	4	2.00	0.48	5.92	0.55	1.08	1.46	293–523	[52]
	2	1.72	0.50	6.00	0.23	0.22	0.09	293–303	[53]
	2	1.90	0.31	5.83	0.37	0.36	0.20	293–303	[47]
	8	2.09	0.49	5.83	0.64	1.10	1.47	293–523	[55]
	46	13.3	13.4	15.0	13.3	13.3	13.3	90–1000	[56]
	124	1.55	2.99	8.44	2.59	0.90	6.64	100–1600	[57]
	68	2.21	1.35	5.62	1.55	2.17	1.04	87–700	[58]
	135	1.53	2.67	7.81	2.21	1.46	1.34	80–1000	[92]
	63	1.60	1.43	6.50	1.13	1.50	0.57	90–500	[93]
	1	1.52	0.66	6.17	0.01	0.00	0.14	300	[94]
	8	1.17	3.04	8.81	2.44	0.64	1.53	298–973	[59]
	11	1.65	1.53	6.50	1.24	1.43	0.56	100–600	[60]
	20	4.41	3.96	8.23	3.19	3.18	3.52	60–1000	[61]
	7	0.85	1.43	7.06	0.82	1.29	2.98	250–1000	[62]
	5	2.19	2.35	7.11	1.97	1.7	1.72	323–523	[95]
	5	0.81	1.48	6.98	0.76	0.58	0.47	298–423	[96]
	4	1.59	1.10	6.34	0.59	0.50	0.38	298–373	[97]
Average	787*	2.75	3.14	7.85	2.84	2.44	3.76		
Krypton	29	3.41	6.47	8.26	3.40	4.00	59.7	50–3273	[26]
	6	2.96	4.24	6.53	1.85	1.84	3.40	100–600	[29]
	1	3.90	1.95	4.82	0.83	0.50	0.91	293	[73]
	2	3.40	2.59	5.36	0.58	0.51	1.53	293–300	[30]
	8	1.70	6.11	7.76	2.28	1.88	3.05	298–973	[64]
	6	1.92	5.77	7.54	2.15	1.83	3.18	298–767	[81]
	8	1.89	6.25	7.86	2.51	2.07	3.20	298–973	[65]
	8	1.88	6.07	7.67	2.25	1.83	2.97	298–973	[35]
	9	1.60	6.61	8.20	2.80	2.40	3.27	298–1151	[31]
	9	1.87	5.82	7.53	2.05	1.71	3.10	298–778	[38]
	6	1.98	5.68	7.45	2.06	1.75	3.09	298–770	[89]
	1	5.59	0.36	3.27	2.47	2.13	0.70	293	[67, 68]
	1	5.08	0.84	3.74	1.97	1.64	0.21	293	[66]
	1	5.42	0.52	3.42	2.30	1.95	0.54	293	[76]
	12	2.01	5.43	7.27	1.83	1.57	2.93	298–773	[98]
	4	2.59	3.19	6.23	1.14	1.28	2.56	237–308	[49]
	2	4.93	0.82	3.82	1.96	1.63	0.43	273–293	[52]
	2	3.80	2.13	4.93	0.70	0.37	1.02	273–293	[54]
	2	3.72	2.10	4.40	0.69	0.68	1.10	273–293	[45, 46]

Table 3: Continued.

Compound	Number of data points	Average RMSD$_r$ in η (%)						ΔT (K)	Reference
		Present study	L-J	Kihara	Lucas	Simsci	Refprop		
	1	4.34	1.49	3.82	1.27	0.90	0.48	293	[47]
	15	2.54	5.66	7.18	2.0	1.87	5.45	293–1600	[56]
	78	2.12	5.77	7.43	2.06	1.69	2.60	300–1300	[57]
	71	4.64	4.98	7.24	3.83	3.77	4.28	119–950	[58]
	235	2.02	6.98	8.64	3.61	3.57	12.5	80–2000	[92]
	51	8.49	7.44	8.66	7.50	7.45	7.40	125–500	[93]
	8	1.86	6.08	7.69	2.26	1.84	2.99	298–973	[59]
	10	4.62	2.00	4.19	2.0	2.09	0.26	150–600	[60]
	26	1.89	6.29	7.95	3.19	3.20	13.4	140–2000	[61]
Average	612*	3.03	6.18	7.94	3.42	3.32	10.2		
Xenon	22	5.51	7.31	5.84	2.10	9.51	12.3	50–973	[26]
	6	5.06	6.39	5.33	1.86	6.59	12.0	100–600	[29]
	17	2.09	4.22	4.46	2.18	1.34	6.71	173–797	[80]
	8	3.13	7.60	5.87	1.42	2.11	7.94	298–973	[35]
	9	3.04	7.43	5.86	1.34	2.24	4.06	298–778	[38]
	7	1.24	2.65	3.75	2.51	0.46	5.94	202–298	[90]
	4	3.75	5.22	6.18	2.20	3.08	2.30	237–308	[49]
	3	0.53	2.62	2.99	2.32	0.74	2.90	273–373	[99]
	2	0.26	2.42	3.24	2.83	0.66	3.45	291	[45, 46]
	9	2.45	6.88	5.27	1.07	1.42	8.06	293–1000	[56]
	41	2.88	7.43	5.61	1.22	1.72	16.1	300–1300	[57]
	67	2.32	5.41	4.68	1.97	1.32	12.0	165–1250	[58]
	130	3.77	6.66	9.69	1.43	3.44	8.68	105–1000	[92]
	47	3.54	5.07	5.27	3.74	3.34	6.56	170–500	[93]
	8	3.11	7.52	5.77	1.60	2.08	7.96	298–973	[59]
	9	1.99	3.64	3.42	3.04	1.80	3.59	200–600	[60]
	14	2.45	5.87	4.93	1.85	1.42	8.25	180–1000	[61]
Average	403*	3.21	6.10	6.57	1.93	2.87	9.44		
Overall	2597**	3.09	5.06	6.92	3.15	3.31	9.19		

*Number of data points for each noble gas. **Total number of data points for all noble gases.

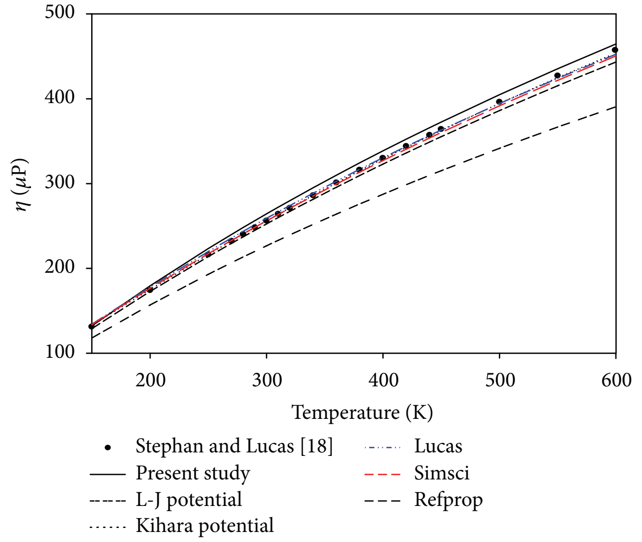

Figure 9: Comparison of measured and calculated viscosities for Kr.

Comparisons of the measured and calculated viscosities for pure noble gases (He, Ne, Ar, Kr, and Xe) are presented in Figures 6, 7, 8, 9, and 10, in order. Using the same set of potential parameters, other 2597 viscosity data available in the literature other than Stephan and Lucas [18] were reproduced with an overall average RMSD$_r$ 3.09% for all noble gases, noting that these results are more accurate than other existing investigations; original Lennard-Jones (12-6) potential 5.06%, Kihara potential with group contribution method 6.92%, Lucas method 3.15%, Simsci correlations 3.31%, and Refprop correlations 9.19%.

It is mentioned here that for each dilute noble gas at 0.1 MPa pressure, the Refprop Database provides selected viscosity data valid in specific temperature ranges, for example, 4–2219 K for helium, 27–1037 K for neon, 87–2992 K for argon, 119–1124 K for krypton, and 164–1100 K for xenon. In this work, their recommended viscosity data were fitted separately for each substance by least-squares analysis to obtain smoothing functions, usually reciprocal temperature expressions of third order, which were used to represent

Table 4: Deviations between experimental and calculated thermal conductivities of pure noble gases.

Compound	Number of points	Average RMSD$_r$ in λ (%)				ΔT (K)	Reference
		Present study	L-J	Simsci	Refprop		
Helium	64	7.77	10.7	2.94	3.52	70–1000	[56]
	8	2.61	5.16	0.78	1.03	298–1010	[31]
	8	2.33	4.40	1.68	1.32	298–973	[34]
	8	2.41	4.42	1.75	1.27	298–973	[36]
	27	5.04	7.95	1.09	1.81	275–725	[57]
	93	6.10	9.10	7.20	20.1	20–1000	[58]
	8	2.47	4.67	1.30	0.95	298–973	[59]
	4	10.2	13.5	4.98	4.16	303–363	[100]
	2	7.72	11.2	2.35	1.25	303	[101]
	25	3.66	6.21	1.41	4.52	50–973	[26]
	6	4.01	6.76	1.19	1.91	100–600	[29]
	11	4.95	7.65	1.44	1.95	100–600	[60]
	29	6.90	9.60	2.50	2.80	80–1000	[102]
	102	6.80	9.50	4.70	12.5	20–1000	[103]
	14	0.41	0.64	0.24	0.31	350–1000	[104]
	6	7.94	11.0	3.37	3.18	303–589	[105]
	52	5.90	8.60	5.50	17.4	20–1000	[106]
	5	11.0	14.0	6.88	7.20	250–600	[62]
	1	5.40	8.76	0.09	1.04	596	[107]
	1	7.24	10.3	1.72	0.53	291	[108]
	4	10.4	13.6	5.11	4.19	308–363	[109]
	2	4.68	7.32	1.32	0.07	302–793	[110]
	1	6.33	9.56	0.92	0.09	311	[111]
	1	6.57	10.0	1.20	0.08	302	[112]
	13	2.16	4.39	1.06	0.29	373–973	[63]
Average	495*	5.90	8.59	3.94	9.47		
Neon	8	1.52	0.62	1.07	2.91	298–973	[64]
	8	2.50	1.16	0.66	3.87	298–973	[65]
	1	1.04	0.54	1.10	2.53	291	[47]
	8	2.74	1.41	0.66	4.11	298–973	[36]
	29	3.50	2.53	0.94	4.11	90–1300	[56]
	44	1.36	0.86	1.65	2.40	275–1275	[57]
	111	2.83	2.65	5.95	12.7	27–1000	[58]
	8	2.55	1.17	0.76	3.92	298–973	[59]
	4	1.67	3.25	2.10	0.84	303–363	[100]
	3	1.25	0.76	1.02	2.14	313–363	[113]
	22	2.40	1.70	2.40	4.36	50–973	[26]
	6	1.81	1.34	1.09	3.25	100–600	[29]
	11	1.48	3.03	2.50	2.04	100–600	[60]
	15	2.92	1.63	0.53	4.01	273–1100	[102]
	111	2.17	2.35	1.59	4.48	27–1500	[114]
	24	2.92	1.41	1.01	5.94	350–1500	[104]
	4	1.39	2.96	1.50	0.37	303–318	[105]
	1	1.36	2.90	1.53	0.14	311	[115]
	1	0.20	1.39	0.32	1.73	296	[107]
	1	1.04	0.53	1.11	2.54	291	[108]
	2	5.86	4.27	4.28	7.50	302–793	[110]
Average	422*	2.41	2.08	2.63	6.20		

Table 4: Continued.

Compound	Number of points	Average RMSD$_r$ in λ (%)					
		Present study	L-J	Simsci	Refprop	ΔT (K)	Reference
Argon	21	2.09	2.72	1.07	1.00	202–394	[90]
	3	2.15	3.97	0.48	5.08	90–273	[108]
	1	1.75	2.95	4.90	4.23	1373	[116]
	1	0.14	4.35	1.09	2.98	291	[47]
	9	1.06	5.27	0.53	1.24	298–1124	[31]
	8	1.21	5.11	0.49	1.17	298–973	[64]
	8	1.53	5.71	0.66	0.99	298–973	[65]
	8	1.48	5.66	0.77	1.09	298–973	[35]
	66	1.76	4.50	1.25	1.60	90–2000	[56]
	14	2.25	6.41	2.36	2.57	331–645	[117]
	97	1.74	4.98	0.80	0.99	280–1390	[57]
	122	2.55	6.17	1.26	5.23	87–3300	[58]
	235	2.10	5.97	1.02	2.20	80–2000	[92]
	63	2.74	3.09	3.08	5.05	90–500	[79]
	63	3.82	4.80	3.40	3.53	90–500	[93]
	8	1.36	5.50	0.54	1.10	298–973	[59]
	3	0.77	4.70	1.37	2.70	313–363	[113]
	29	2.63	5.64	2.48	7.10	50–3273	[26]
	6	1.92	4.11	2.46	5.20	100–600	[29]
	11	1.65	3.37	1.39	3.07	100–600	[60]
	54	2.02	5.78	1.07	2.55	80–2000	[102]
	118	1.67	4.82	1.21	2.14	88–2500	[103]
	24	1.70	6.20	0.50	0.90	350–1500	[104]
	4	2.73	3.57	1.65	0.77	273–593	[105]
	4	0.49	4.15	0.68	2.20	308–363	[118]
	3	1.08	3.52	0.21	1.81	300–340	[119]
	8	0.79	4.42	1.20	2.51	295–420	[120]
	60	2.03	4.95	1.16	2.04	90–2000	[106]
	7	1.41	3.86	1.09	1.43	250–1000	[62]
	1	1.40	3.19	0.25	1.52	311	[115]
	1	1.14	3.41	0.06	1.93	296	[107]
	4	0.50	4.15	0.67	2.20	308–363	[109]
	2	3.10	7.10	2.40	2.70	302–793	[110]
	1	1.40	3.20	0.25	1.52	311	[111]
	22	1.46	4.21	0.84	3.31	87–1000	[29]
Average	1089*	2.11	5.22	1.31	2.82		
Krypton	9	1.90	14.8	0.82	2.93	298–1149	[31]
	8	1.80	14.8	0.88	3.10	298–973	[64]
	8	1.65	15.1	1.24	3.44	298–973	[65]
	18	3.20	19.5	4.18	6.57	125–1300	[56]
	5	4.88	10.6	1.94	0.94	291–318	[57]
	101	2.33	14.0	1.71	3.19	119–1900	[58]
	6	3.12	13.4	2.25	3.45	100–600	[26]
	235	2.60	15.5	2.50	4.50	80–2000	[92]
	51	2.50	12.5	0.96	2.50	125–500	[93]
	8	1.75	14.9	1.10	3.28	298–973	[59]
	3	0.81	15.5	3.68	5.50	313–363	[113]
	27	3.50	14.6	2.70	7.74	50–2273	[26]
	10	4.62	10.8	2.46	0.64	150–600	[60]
	109	5.80	14.4	5.33	6.25	120–2000	[114]

Table 4: Continued.

Compound	Number of points	Average RMSD_r in λ (%)				ΔT (K)	Reference
		Present study	L-J	Simsci	Refprop		
	24	3.00	15.9	2.50	3.50	350–1500	[104]
	5	5.76	9.80	2.67	0.78	303–318	[105]
	4	4.24	11.3	1.35	1.06	308–363	[118]
	1	4.38	11.0	1.30	0.65	311	[115]
	1	4.16	10.9	1.17	0.81	291	[108]
	4	4.21	11.3	1.34	1.11	308–363	[109]
	2	4.06	17.4	5.03	6.98	302–793	[110]
Average	639*	3.22	14.7	2.70	4.35		
Xenon	7	1.29	14.2	9.68	2.32	202–298	[90]
	8	3.28	14.2	2.65	1.43	298–973	[35]
	24	7.30	17.7	1.02	4.55	175–1300	[56]
	1	3.53	12.7	0.60	1.95	291	[57]
	1	3.36	12.6	0.77	1.78	291	[108]
	134	5.36	15.7	5.80	10.1	165–5000	[58]
	230	4.87	15.3	4.83	1.96	105–2000	[92]
	47	3.33	12.0	2.10	0.71	170–500	[93]
	8	3.29	14.2	2.64	1.43	298–973	[59]
	4	3.39	13.1	0.57	2.48	303–363	[100]
	3	8.35	17.6	4.75	7.55	313–363	[113]
	29	5.84	14.9	8.18	2.90	50–3273	[26]
	6	5.50	12.8	5.96	2.82	100–600	[29]
	9	1.46	11.2	3.60	0.92	200–600	[60]
	95	6.40	16.7	1.74	3.93	165–1500	[114]
	24	8.00	19.0	1.20	5.10	350–1500	[104]
	6	4.20	7.60	7.87	5.20	303–318	[105]
	67	5.64	16.1	5.97	10.2	165–5000	[106]
	2	9.00	19.0	3.90	7.01	302–793	[110]
	1	0.80	9.10	4.95	2.06	311	[111]
	1	7.30	16.3	3.43	6.00	302	[112]
Average	707*	5.26	15.4	4.39	4.76		
Overall	3352**	3.59	9.28	2.78	4.93		

*Number of data points for each noble gas. **Total number of data points for all noble gases.

viscosity data at the same temperature as those of experimental data for the reasonable comparisons. Prediction results from the Refprop correlations are observed to be not in reliable agreement with measured viscosity data, especially near upper and lower limits of temperature ranges specified previously, as shown in Table 3. The Simsci Database [24] provides the smoothing viscosity function with four coefficients c_i ($i = 1$ to 4)

$$\eta = \frac{c_1 T^{c_2}}{\left(1 + c_3/T + c_4/T\right)} \qquad (24)$$

valid in specific temperature ranges: 20–2000 K for helium, 30–3272 K for neon, 83–3273 K for argon, 100–1500 K for krypton, and 100–1600 K for xenon.

The next stage of this work is to calculate other properties such as thermal conductivity and self-diffusion coefficient, not used for parameter determinations, using the same set of potential parameters determined earlier. As shown in Table 4, the overall average RMSD_r value of 3.59% between a total of 3352 experimental and calculated thermal conductivities obtained by the proposed model is somewhat less reliable to the Simsci correlations 2.78%, but compares very well with the original Lennard-Jones (12-6) potential 9.28% and the Refprop correlations 4.93%.

Like the case of viscosities, the Refprop Database [22] provides dilute gas thermal conductivity data at 0.1 MPa suitable in specific temperature ranges: 4–1100 K for helium, 27–1039 K for neon, 87–2968 K for argon, 119–1100 K for krypton, and 164–1101 K for xenon. The procedure to produce thermal conductivity data is the same as that of viscosity. The Simsci Database also provides the same type of soothing thermal conductivity function, (24), in specific temperature ranges: 30–2000 K for helium, 30–3272 K for neon, 90–3273 K for argon, 120–2000 K for krypton, and 165–1500 K for xenon. Comparisons of the measured and calculated thermal conductivities for pure noble gases (He, Ne, Ar,

Table 5: Deviations between experimental and calculated self-diffusion coefficients of pure noble gases.

Compound	Number of points	Average RMSD$_r$ in D (%)			ΔT (K)	Reference
		Present study	L-J	Fuller		
		Prediction results				
Helium	17	4.72	2.04	10.6	50–623	[26]
	7	11.0	8.44	13.1	14–296	[56]
Average	*24**	*6.55*	*3.90*	*11.3*		
Neon	29	3.36	2.25	8.07	50–3273	[26]
	17	6.85	4.93	13.2	77–6000	[56]
	20	4.72	2.78	6.50	295–1219	[121]
	1	4.55	7.77	5.96	293	[122]
Average	*67**	*4.67*	*3.17*	*8.88*		
Argon	29	2.87	4.70	10.9	50–323	[26]
	12	4.10	3.51	14.2	90–326	[56]
Average	*41**	*3.23*	*4.35*	*11.9*		
Krypton	29	4.00	13.92	9.70	50–3273	[26]
	18	6.83	16.93	3.69	199–6000	[56]
	1	4.90	8.94	3.30	293	[123]
Average	*48**	*5.08*	*14.95*	*7.31*		
Xenon	29	6.27	13.9	16.2	50–3273	[26]
	27	6.02	16.9	13.1	194–15000	[56]
	1	1.06	7.40	17.2	293	[123]
Average	*57**	*6.06*	*15.2*	*14.8*		
Overall	237**	5.03	8.73	10.7		

*Number of data points for each noble gas. **Total number of data points for all noble gases.

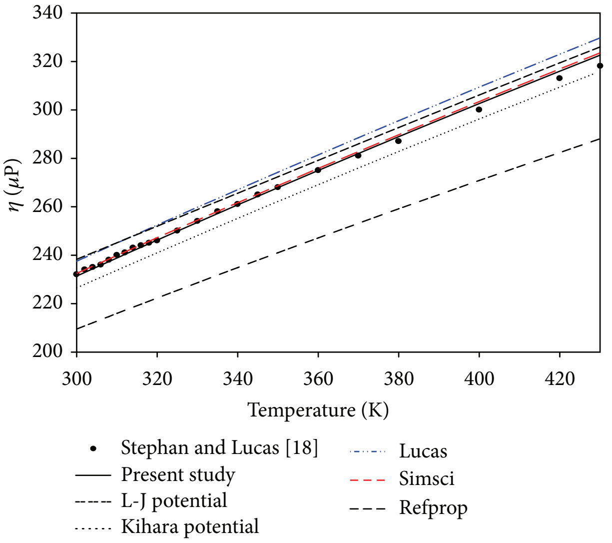

Figure 10: Comparison of measured and calculated viscosities for Xe.

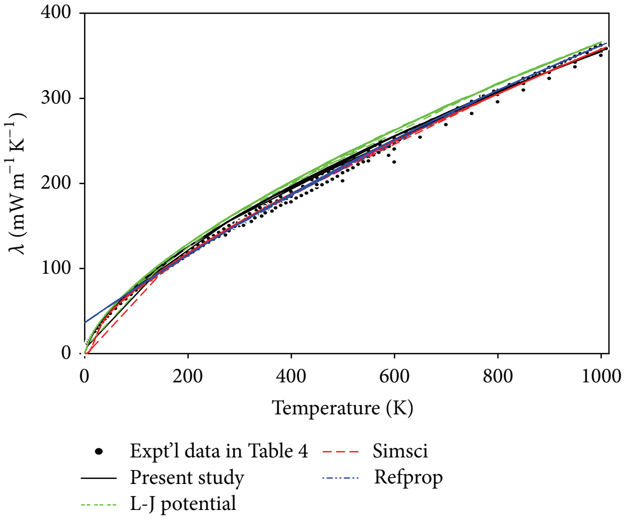

Figure 11: Comparison of measured and calculated thermal conductivities for He.

Kr, and Xe) are depicted in Figures 11, 12, 13, 14, and 15, in order. As shown in Figures 14 and 15, Refprop Database shows considerably larger discrepancies between measured and calculated thermal conductivities for krypton and xenon than other methods particularly at high-temperature region, at which recommended data is not reliable, as specified by them.

A total of 237 self-diffusion coefficient data were next tested. As shown in Table 5, the overall average RMSD$_r$ value of 5.03% from all noble gases was obtained by this work, in which the result is in better agreement with experimental data than those of the original Lennard-Jones (12-6) potential 8.73% and of the Fuller method [25] 10.7%. It is indicated that for the helium and neon gas, the proposed method is less

Table 6: Deviations between experimental and predicted second cross-virial coefficients of noble gas mixtures.

Mixtures	Number of points	Average RMSD in B_{12} ($\mathrm{cm^3\,mol^{-1}}$)				ΔT (K)	Reference
		Present study	L-J	Dymond et al.	Tsonopoulos		
		Mixtures of noble gases					
Helium-neon	18	2.05	5.82	0.94	9.40	15–323	[2]
	23	0.66	0.54	1.72	10.6	273–3273	[26]
Helium-argon	21	2.03	0.92	0.44	6.85	90–773	[2]
	23	4.90	5.71	6.37	14.8	273–3273	[26]
Helium-krypton	15	5.66	3.49	0.99	1.84	90–323	[2]
	23	8.54	12.0	12.0	15.9	273–3273	[26]
Helium-xenon	9	10.9	6.07	0.71	7.14	120–323	[2]
	23	15.8	19.7	23.3	21.5	273–3273	[26]
Average	*155**	*6.15*	*7.12*	*6.75*	*11.9*		
Neon-argon	30	1.68	34.9	1.00	7.72	84–475	[2]
	23	3.15	1.15	6.69	4.71	273–3273	[26]
Neon-krypton	48	5.15	48.6	2.76	14.3	100–475	[2]
	23	3.86	3.29	8.07	6.69	273–3273	[26]
Neon-xenon	28	16.5	39.4	2.61	17.6	162–475	[2]
	23	10.8	7.36	18.9	12.5	273–3273	[26]
Average	*175**	*6.68*	*27.2*	*5.77*	*11.2*		
Argon-krypton	50	3.26	150.3	1.82	2.51	108–695	[2]
	23	1.58	16.7	2.93	4.53	273–3273	[26]
Argon-xenon	5	12.3	125.5	0.29	12.1	173–323	[2]
	23	4.60	23.9	30.0	5.76	273–3273	[26]
Average	*101**	*3.63*	*89.9*	*8.43*	*4.18*		
Krypton-xenon	35	7.34	173.7	1.97	5.76	160–700	[2]
	23	2.34	42.6	3.40	4.44	273–3273	[26]
Average	*58**	*5.36*	*121.7*	*2.54*	*5.24*		
Overall	489**	5.73	45.0	6.25	9.28		

*Number of data points for each gas mixture. **Total number of data points for all gas mixtures.

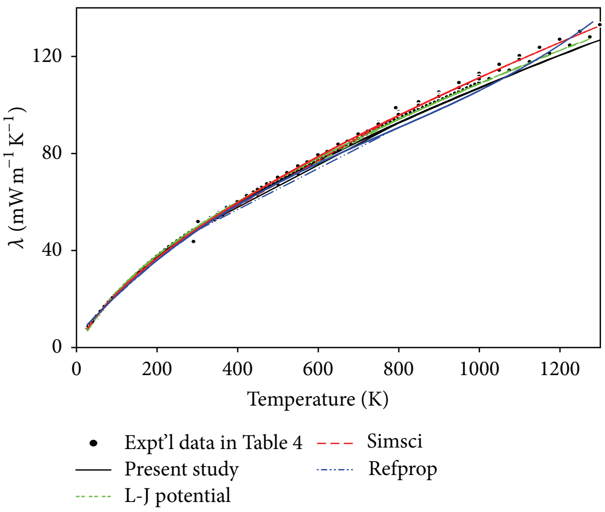

Figure 12: Comparison of measured and calculated thermal conductivities for Ne.

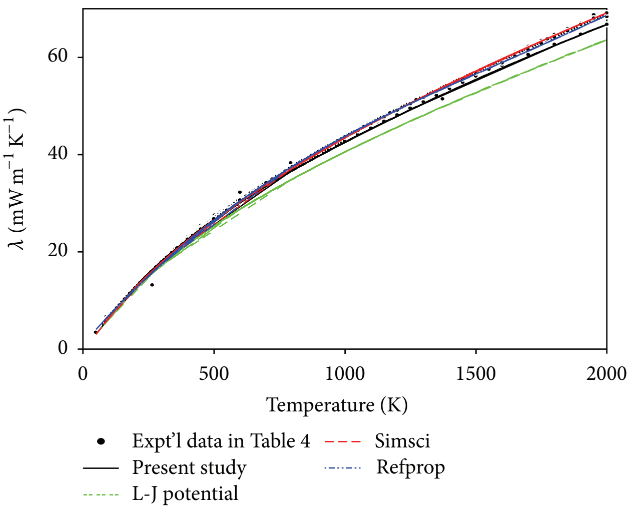

Figure 13: Comparison of measured and calculated thermal conductivities for Ar.

accurate than the original Lennard-Jones (12-6) potential. Comparisons of the measured and calculated self-diffusion coefficients for noble gases (He, Ne, Ar, Kr, and Xe) are depicted in Figures 16, 17, 18, 19, and 20, in order.

Table 7: Deviations between experimental and predicted mixture viscosities of noble gas mixtures.

Mixtures	Number of points	Average RMSD$_r$ in η_{mix} (%)			ΔT (K)	Reference
		Present study	L-J	Lucas method		
Helium-neon	87	6.24	13.6	8.85	50–3273	[26]
	7	2.40	4.87	3.56	291	[47]
	10	1.93	4.93	4.39	293	[53]
	32	1.75	4.77	8.18	298–973	[36]
	3	2.31	4.88	3.97	293	[40–42]
	10	2.58	5.15	3.80	293–523	[124]
	11	3.36	4.82	6.98	293–523	[55]
	31	2.22	4.96	3.67	20–523	[56]
	162	2.10	8.40	7.49	100–950	[57]
Helium-argon	87	4.49	7.31	4.95	50–3273	[26]
	12	3.38	4.25	3.51	293–303	[125]
	11	3.75	3.66	4.78	291	[47]
	58	3.84	4.07	4.76	72–192	[50]
	40	2.98	6.06	3.63	298–993	[31]
	3	3.52	0.92	6.46	293	[78]
	3	4.09	3.01	5.19	293	[40–42]
	6	3.69	3.12	5.25	293–523	[55]
	16	6.72	7.04	5.47	293–523	[56]
	123	1.29	5.18	3.20	100–1500	[57]
	28	3.14	3.23	4.45	298	[126]
	12	1.26	2.44	4.57	300–1100	[127]
	6	3.62	0.51	7.15	298	[128]
Helium-krypton	87	4.60	9.41	13.4	50–3273	[26]
	9	4.44	7.72	9.63	291	[45, 46]
	16	4.98	5.28	10.5	303	[54]
	40	7.72	8.91	5.78	298–993	[31]
	135	4.07	11.8	4.94	300–1000	[57]
Helium-xenon	87	3.85	9.63	13.9	50–3273	[26]
	10	3.41	6.11	19.2	291	[45, 46]
	18	2.50	8.85	13.6	298–778	[38]
	90	2.34	9.46	12.7	300–750	[57]
Average	1250*	3.52	8.34	8.33		
Neon-argon	87	1.91	3.95	4.23	50–3273	[26]
	6	1.24	2.80	1.60	293	[53]
	36	0.66	2.15	2.85	298–973	[64]
	26	3.87	4.34	4.24	72–291	[77]
	3	1.68	1.48	0.70	293	[78]
	3	1.61	0.95	0.66	293	[40–42]
	9	1.43	1.85	0.70	291	[47]
	12	3.22	3.95	3.56	293–523	[55]
	16	2.56	1.59	1.14	293–523	[56]
	162	0.95	4.28	2.72	100–950	[57]
Neon-krypton	87	2.63	10.3	3.25	50–3273	[26]
	9	1.28	8.04	2.44	291	[45, 46]
	40	0.85	9.63	1.60	298–973	[65]
	126	0.78	10.5	1.55	300–950	[57]

Table 7: Continued.

Mixtures	Number of points	Average RMSD$_r$ in η_{mix} (%)			ΔT (K)	Reference
		Present study	L-J	Lucas method		
Neon-xenon	87	4.70	11.1	3.94	50–3273	[26]
	8	0.85	7.30	6.42	291	[45, 46]
	12	2.46	8.69	3.74	298–773	[38]
	90	4.70	10.2	3.11	300–750	[57]
Average	819*	2.46	8.11	2.95		
Argon-krypton	87	2.69	10.7	3.13	50–3273	[26]
	36	0.71	10.5	1.81	298–973	[64]
	8	2.20	8.40	1.76	291	[45, 46]
	189	0.97	10.8	2.30	300–1300	[57]
Argon-xenon	87	4.07	11.3	2.84	50–3273	[26]
	9	0.64	8.04	4.01	291	[45, 46]
	12	1.87	9.15	1.61	298–773	[38]
	34	2.46	10.5	2.62	173–299	[80]
	189	2.71	13.2	1.42	173–1597	[57]
Average	651*	2.20	11.4	2.23		
Krypton-xenon	87	3.97	14.5	2.71	50–3273	[26]
	9	1.22	11.2	2.19	291	[45, 46]
	12	2.18	14.1	1.18	298–773	[38]
	90	3.52	14.7	2.98	300–750	[57]
Average	198*	3.53	14.4	2.72		
Overall	2918**	2.93	10.6	4.05		

*Number of data points for each gas mixture. **Total number of data points for all gas mixtures.

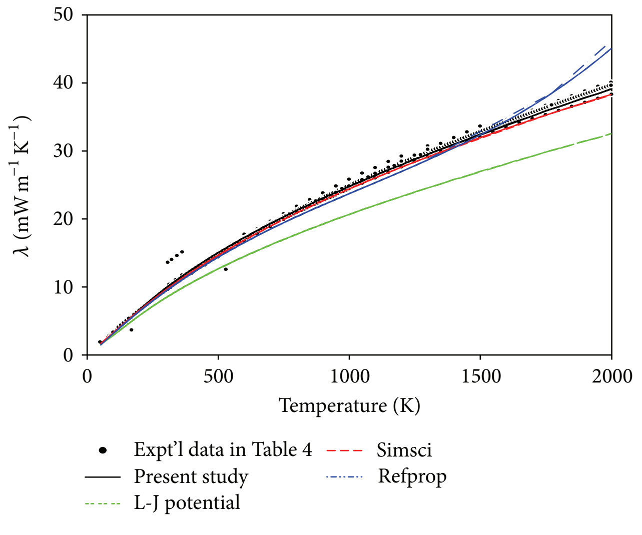

Figure 14: Comparison of measured and calculated thermal conductivities for Kr.

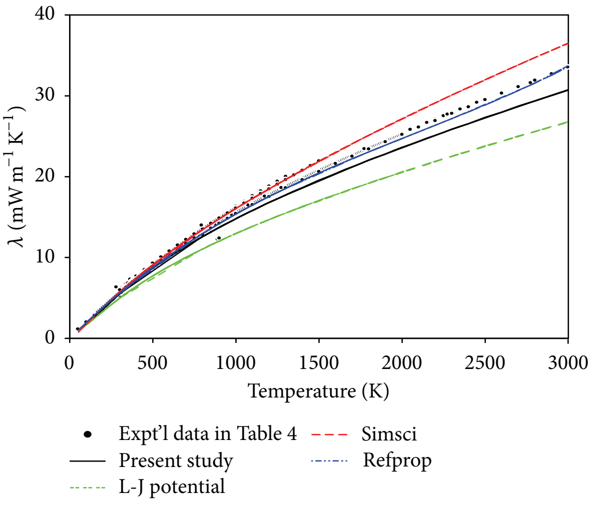

Figure 15: Comparison of measured and calculated thermal conductivities for Xe.

3.2. Noble Gas Mixtures. The same set of potential parameters estimated from pure gas information was applied to predict mixture properties such as second cross-virial coefficient, mixture viscosity, mixture thermal conductivity, and binary diffusion coefficient with no additional parameters.

Table 6 shows that for the second cross-virial coefficient calculations, a total of 489 data of noble gas mixtures taken from the critical compilation of Dymond et al. [17] and from the Kestin et al. [26] were fitted to be overall average RMSD value of 5.73 cm^3 mol^{-1}, while the 6.25 cm^3 mol^{-1} value was obtained by the smoothing functions of Dymond et al. in the same fashion as used in the pure gas calculations. And the 45.0 and 9.28 cm^3 mol^{-1} RMSD values were found by the original Lennard-Jones (12-6) potential and the

Table 8: Deviations between experimental and predicted thermal conductivities of noble gas mixtures.

Mixtures	Number of points	Average RMSD$_r$ in λ_{mix} (%)			ΔT (K)	Reference
		Present study	L-J	Wassiljewa[a]		
Helium-neon	32	9.69	12.2	5.98	298–973	[36]
	7	2.30	4.68	1.59	291	[47]
	138	5.62	8.08	3.14	275–1175	[57]
	12	11.2	13.9	7.17	303–363	[100]
	15	8.59	11.3	3.73	350–1050	[104]
	66	7.65	10.1	4.28	50–973	[26]
	7	12.6	12.2	6.08	298	[107]
	8	7.14	7.62	6.27	302–793	[110]
Helium-argon	32	15.2	14.4	10.8	298–993	[31]
	20	8.61	9.59	12.1	291	[47]
	4	12.9	12.2	8.31	273	[56]
	138	9.00	7.94	5.22	275–1025	[57]
	15	10.8	9.46	5.98	350–1050	[104]
	66	8.16	7.22	3.91	50–973	[26]
	9	9.20	8.23	4.99	298	[107]
	12	12.3	11.8	7.54	308–363	[109]
	8	10.6	10.5	11.6	302–793	[110]
	5	10.3	9.99	5.79	311	[111]
	4	9.21	8.76	6.80	273	[129]
Helium-krypton	6	8.47	6.24	3.27	302	[112]
	32	9.82	6.11	4.16	298–993	[31]
	9	5.00	3.12	1.88	291	[57]
	15	9.92	5.27	4.18	350–1050	[104]
	66	8.76	5.81	3.68	50–973	[26]
	9	5.39	3.09	2.29	291	[45, 46]
	16	10.1	9.50	4.52	308–363	[109]
	12	6.23	5.49	4.16	302–793	[110]
Helium-xenon	4	3.95	8.95	1.97	302	[112]
	16	4.57	7.00	3.52	303–363	[100]
	15	1.54	4.05	2.62	350–1050	[104]
	66	7.19	8.93	4.22	50–973	[26]
	10	6.19	10.02	3.61	291	[45, 46]
	8	4.17	8.2	3.43	302–793	[110]
	6	4.35	9.3	2.24	311	[111]
Average	888*	8.11	8.42	4.73		
Neon-argon	32	3.82	4.91	4.91	298–973	[64]
	9	3.59	5.91	5.08	291	[47]
	12	2.87	5.15	4.36	313–363	[113]
	24	3.51	5.70	6.54	350–1500	[104]
	87	2.65	4.62	5.34	50–3273	[26]
	11	0.84	2.23	1.17	311	[115]
	8	0.77	2.64	2.12	298	[107]
	8	5.22	7.33	7.34	302–793	[110]
Neon-krypton	32	1.37	4.94	2.10	298–973	[65]
	198	25.7	32.2	28.1	275–1275	[57]
	12	0.97	8.51	2.26	313–363	[113]
	24	15.8	23.6	19.2	350–1500	[104]
	87	3.35	7.55	2.58	50–3273	[26]
	9	4.04	5.58	1.54	311	[115]
	9	3.85	5.28	2.34	291	[45, 46]
	6	6.10	10.4	6.27	302–793	[110]

Table 8: Continued.

Mixtures	Number of points	Average RMSD_r in λ_{mix} (%)			ΔT (K)	Reference
		Present study	L-J	Wassiljewa[a]		
Neon-xenon	9	2.11	4.50	2.18	291	[57]
	12	5.24	8.08	4.49	303–363	[100]
	24	4.52	7.59	5.03	350–1500	[104]
	87	4.41	5.24	2.43	50–3273	[26]
	9	1.90	4.42	2.04	291	[45, 46]
	6	6.00	8.72	6.06	302–793	[110]
Average	715*	9.94	13.7	11.0		
Argon-krypton	32	1.14	10.3	2.42	298–973	[64]
	9	5.65	5.02	3.31	291	[57]
	24	2.11	9.69	2.51	350–1500	[104]
	87	2.73	10.1	3.32	50–3273	[26]
	6	4.70	5.58	2.46	311	[115]
	8	5.77	5.28	3.58	291	[45, 46]
	12	3.52	7.30	1.50	308–363	[109]
	6	3.32	13.2	5.55	302–793	[110]
Argon-xenon	9	2.63	5.59	2.94	291	[57]
	8	10.5	17.1	10.0	311–366	[113]
	24	1.14	8.46	1.38	350–1500	[104]
	87	3.10	8.11	2.34	50–3273	[26]
	9	2.87	5.43	3.19	291	[45, 46]
	6	3.43	10.8	3.14	302–793	[110]
	6	4.05	4.03	4.94	311	[111]
Average	333*	2.97	8.90	2.92		
Krypton-xenon	5	4.42	14.9	3.91	302	[112]
	9	1.87	12.5	1.03	291	[57]
	12	7.14	18.3	7.24	313–363	[113]
	24	2.35	13.7	2.37	350–1500	[104]
	87	5.13	16.0	3.97	50–3273	[26]
	9	1.76	12.4	0.92	291	[45, 46]
	10	6.06	17.5	5.90	302–793	[110]
Average	156*	4.51	15.5	3.75		
Overall	2092**	7.65	10.8	6.50		

[*] Number of data points for each mixture.

[**] Total number of data points for all gas mixture mixtures.

[a] Wassiljewa equation [15] with the combinational factor of Mason and Saxena [16].

corresponding states method of Tsonopoulos, respectively. A comparison of measured and calculated second cross-virial coefficients of Ar + Kr mixture is shown in Figure 21.

Prediction results of noble gas mixture viscosities are presented in Table 7. A total of 2918 viscosity data points for all noble gas mixtures were calculated in this paper, indicating that the present study is in better agreement between experimental and calculated data than other methods on a %RMSD_r criterion: 2.93% by the present model, 10.6% by the original Lennard-Jones (12-6) potential, and 4.05% by the Lucas method. However, it is noted that for krypton and xenon mixture, this work is less reliable to the Lucas method. Figure 22 shows the comparison of measured and calculated viscosities of He + Ne mixture.

Given in Table 8 are the resulting %RMSD_r values between a total of 2092 measured and predicted mixture thermal conductivity data. Based on the overall average %RMSD_r value of all noble gas mixtures, 7.65% of the present study is in slightly worse agreement between measured and predicted mixture thermal conductivities than 6.50% of the Wassiljewa equation [15] with the combinational factor of Mason and Saxena [16] and is more feasible to 10.8% of the original Lennard-Jones (12-6) potential. A comparison of measured and calculated thermal conductivities of Ne + Kr mixture is shown in Figure 23.

Included in Table 9 are the resulting %RMSD_r values between a total of 1240 measured and predicted binary diffusion coefficient data for noble gas mixtures, in which 4.98 %RMSD_r of the present study is in quite better agreement between measured and predicted binary diffusion coefficients than 7.95 %RMSD_r of the original Lennard-Jones (12-6) potential and 6.24 %RMSD_r of the Fuller method.

Table 9: Deviations between experimental and predicted binary diffusion coefficients of noble gas mixtures.

Compound	Number of points	Average RMSD$_r$ in D (%)				
		Present study	L-J	Fuller	ΔT (K)	Reference
Helium-neon	26	2.45	3.77	10.6	50–1773	[26]
	7	1.04	3.09	8.31	200–673	[29]
	1	5.20	1.32	12.7	1000	[130]
	5	2.01	6.19	3.52	65–295	[131]
	6	3.52	1.03	9.42	298–973	[36]
	26	9.89	7.35	5.09	200–1250	[132]
	20	5.27	4.93	12.7	297–1268	[121]
	1	14.0	10.6	8.99	293	[133]
	14	2.81	5.29	7.79	273–683	[56]
Helium-argon	29	2.35	2.72	7.04	50–3273	[26]
	7	0.56	0.12	4.91	200–673	[29]
	1	8.91	8.18	0.77	1000	[130]
	3	3.15	4.11	2.93	276–346	[134]
	8	2.78	3.57	4.06	298–498	[135]
	1	1.66	2.67	0.67	298	[136]
	1	0.91	0.08	1.87	298	[137]
	3	3.84	3.71	2.87	287–418	[138]
	6	8.30	7.80	1.68	298–1100	[139]
	1	1.21	2.22	0.17	296	[140]
	1	0.58	1.63	1.11	273	[12]
	1	1.69	2.75	0.01	273	[55]
	2	5.42	4.92	4.23	276–418	[18]
	4	1.37	2.84	2.76	90–400	[131]
	14	2.63	2.50	2.65	251–418	[141]
	17	5.01	5.08	3.39	276–1100	[142]
	8	5.69	5.05	0.65	298–993	[31]
	26	6.02	5.59	2.13	200–1250	[132]
	21	9.66	8.79	6.62	298–1272	[121]
	84	8.65	8.68	5.25	118–4500	[56]
Helium-krypton	29	2.60	7.00	5.51	50–3273	[26]
	7	2.44	5.18	6.12	200–673	[29]
	1	0.88	8.40	0.34	1000	[130]
	4	14.2	17.0	18.6	111–400	[131]
	8	2.04	7.40	4.22	298–993	[31]
	26	5.12	2.86	3.41	200–940	[132]
	21	5.32	12.4	8.11	307–1274	[121]
	4	3.48	4.02	6.69	273–318	[56]
Helium-xenon	29	7.21	13.1	5.35	50–3273	[26]
	7	5.13	11.8	4.80	200–673	[29]
	1	11.0	17.5	2.85	1000	[130]
	4	6.21	12.6	6.93	169–400	[131]
	6	1.69	8.48	3.59	298–778	[38]
	26	9.4	15.6	4.93	200–940	[132]
	21	9.96	16.3	6.65	297–1270	[121]
	8	7.6	13.5	8.01	273–394	[56]
	10	2.2	8.97	2.82	220–400	[143]
	2	2.3	9.1	2.97	273–315	[144]
Average	557*	5.80	7.61	5.72		

Table 9: Continued.

Compound	Number of points	Average RMSD$_r$ in D (%)			ΔT (K)	Reference
		Present study	L-J	Fuller		
Neon-argon	29	2.03	3.08	5.38	50–3273	[26]
	7	1.64	2.83	2.25	200–673	[29]
	1	3.38	6.84	1.17	1000	[130]
	4	2.60	3.14	3.36	90–400	[131]
	8	0.76	3.61	2.50	298–973	[64]
	5	5.42	1.66	4.03	90–473	[145]
	4	2.77	1.72	2.10	273–318	[146]
	26	1.86	3.76	1.51	200–940	[132]
	20	5.89	7.29	4.91	297–1274	[121]
	1	3.21	7.39	7.77	293	[147, 148]
	19	3.15	3.25	3.52	194–680	[56]
	5	5.47	0.79	1.06	277–365	[149]
Neon-krypton	29	2.06	10.4	6.99	50–3273	[26]
	7	2.31	10.4	8.25	200–673	[29]
	1	0.58	12.3	4.19	1000	[130]
	4	4.37	9.32	6.83	111–400	[131]
	4	6.11	7.25	6.32	273–318	[146]
	8	2.75	9.80	5.78	298–973	[65]
	26	3.73	13.0	8.44	200–940	[132]
	20	5.72	9.45	5.31	269–1270	[121]
	4	6.11	7.25	6.32	273–318	[56]
Neon-xenon	29	5.49	11.8	6.50	50–3273	[26]
	7	4.82	11.9	7.49	200–673	[29]
	1	6.22	13.3	3.79	1000	[130]
	4	4.09	11.1	6.82	169–400	[131]
	6	2.03	9.38	4.24	298–773	[38]
	26	6.97	7.81	7.58	200–940	[132]
	21	8.96	15.5	9.15	297–1270	[121]
	4	1.14	8.37	4.82	273–318	[56]
	5	5.59	12.6	9.16	275–362	[149]
Average	335*	4.15	8.18	5.73		
Argon-krypton	29	3.49	7.91	10.0	50–3273	[26]
	7	2.37	6.02	4.28	200–673	[29]
	1	0.08	8.05	0.37	1000	[130]
	1	0.33	7.03	0.26	273	[18]
	4	2.26	4.42	5.99	169–400	[131]
	8	8.60	5.25	19.2	77–600	[150]
	9	4.01	7.89	3.39	199–473	[142]
	5	5.85	8.91	5.25	273–473	[145]
	4	3.85	3.69	2.98	273–318	[146]
	8	1.87	8.82	3.42	298–973	[64]
	11	2.23	4.79	2.89	200–400	[151]
	26	9.30	15.3	10.6	200–940	[132]
	21	2.88	9.59	4.20	300–1274	[121]
	13	3.51	7.89	3.37	199–407	[56]
Argon-xenon	29	5.48	8.62	11.5	50–3273	[26]
	7	2.46	6.39	6.68	200–673	[29]
	1	7.99	13.0	3.23	1000	[130]

Table 9: Continued.

Compound	Number of points	Average RMSD$_r$ in D (%)			ΔT (K)	Reference
		Present study	L-J	Fuller		
	2	5.72	6.25	6.34	195–378	[18]
	4	2.43	5.43	10.6	169–400	[131]
	4	3.16	6.25	6.88	194–378	[152]
	6	1.86	6.41	3.16	298–773	[38]
	26	5.57	9.95	4.59	200–940	[132]
	21	4.18	7.51	5.35	298–1272	[121]
	19	3.79	7.11	9.07	173–1597	[153]
	13	3.93	6.96	5.83	194–394	[56]
Average	279*	4.48	8.42	7.16		
Krypton-xenon	29	4.46	7.05	12.1	50–3273	[26]
	7	1.38	4.42	7.54	200–673	[29]
	1	4.70	10.5	4.63	1000	[130]
	4	1.38	3.27	12.2	169–400	[131]
	6	1.10	4.72	2.88	298–773	[38]
	22	7.00	11.1	7.52	297–1270	[121]
Average	69*	4.49	7.70	9.27		
Overall	1240**	4.98	7.95	6.24		

*Number of data points for each mixture. **Total number of data points for all gas mixtures.

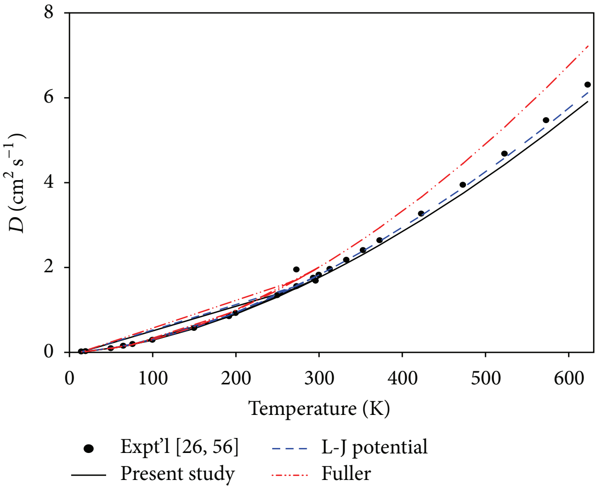

Figure 16: Comparison of measured and calculated self-diffusion coefficients for He.

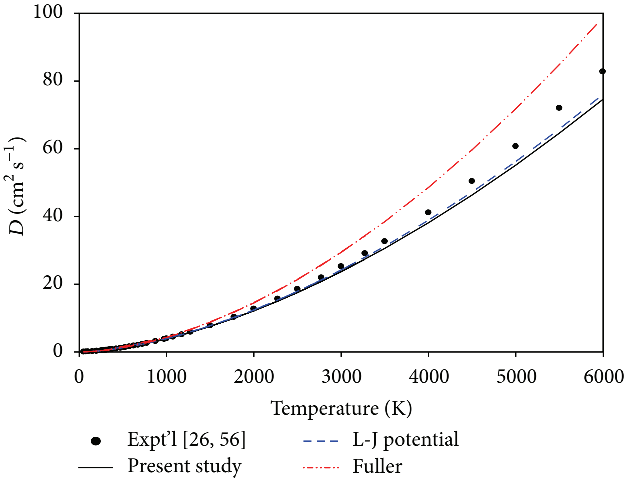

Figure 17: Comparison of measured and calculated self-diffusion coefficients for Ne.

A comparison of measured and calculated binary diffusion coefficients for He + Ne mixture is shown in Figure 24.

4. Conclusions

The three-parameter Lennard-Jones (12-6) potential function has been empirically modified by introducing a temperature-correction parameter to the reduced temperature T^* for the calculation of the thermodynamic property (second virial coefficient) and dilute transport properties (viscosity, thermal conductivity, and diffusion coefficient) of noble gases (He, Ne, Ar, Kr, and Xe) and their binary mixtures. Separately for each species, a single set of three potential parameters (σ, ε, and τ) is estimated when the second virial coefficient and viscosity data are regressed together within the experimental errors. Obtained potential parameters are used to reproduce second virial coefficient and viscosity data and in all following predictions of other properties like thermal conductivity and diffusion coefficient. Noble gas mixture properties are calculated with the same set of parameters as well.

For the second virial coefficient calculations of pure noble gases, the three-parameter Lennard-Jones (12-6) potential proposed in this paper is quite comparable to Dymond's correlations and produces more accurate results than the original two-parameter Lennard-Jones (12-6) potential, the

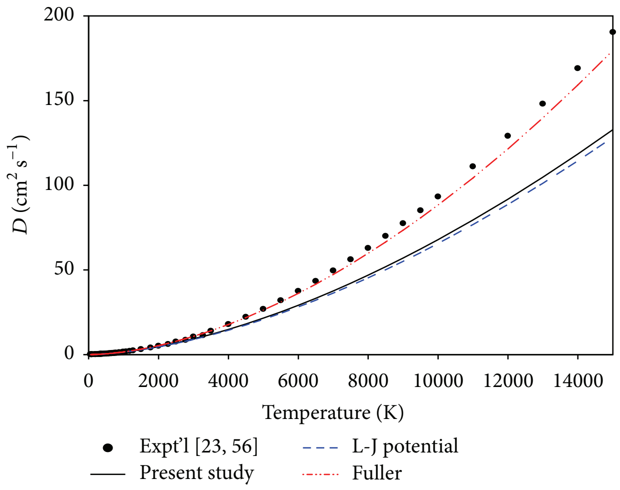

Figure 18: Comparison of measured and calculated self-diffusion coefficients for Ar.

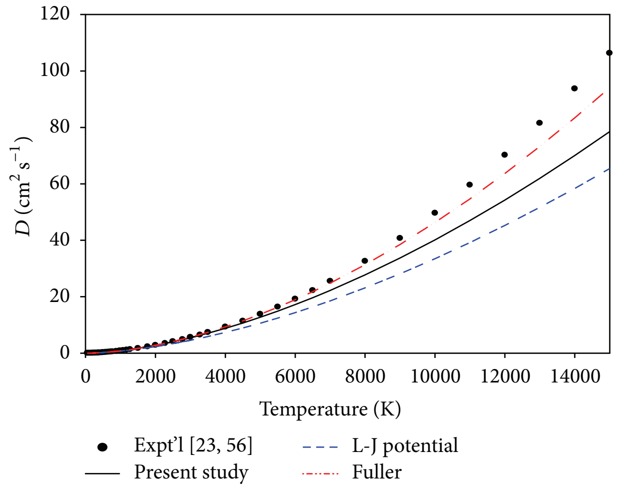

Figure 19: Comparison of measured and calculated self-diffusion coefficients for Kr.

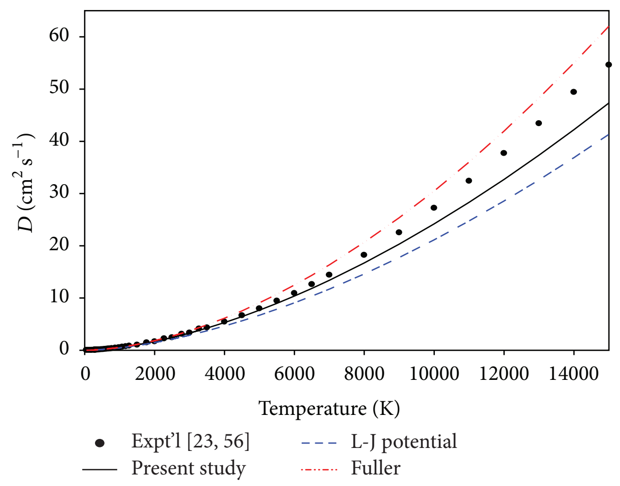

Figure 20: Comparison of measured and calculated self-diffusion coefficients for Xe.

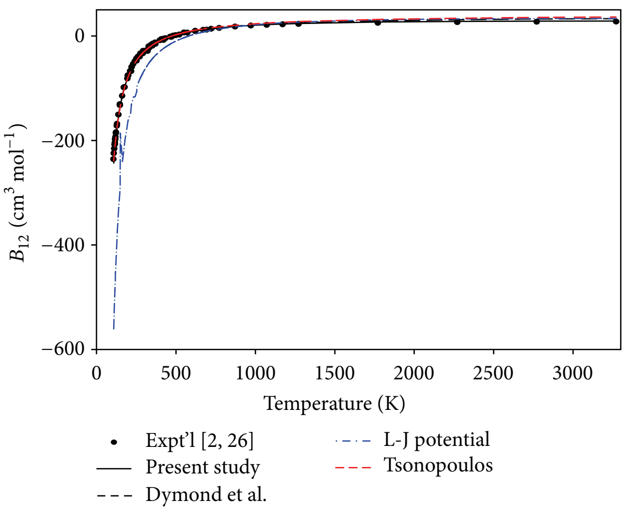

Figure 21: Comparison of measured and calculated second cross-virial coefficients for Ar + Kr mixture.

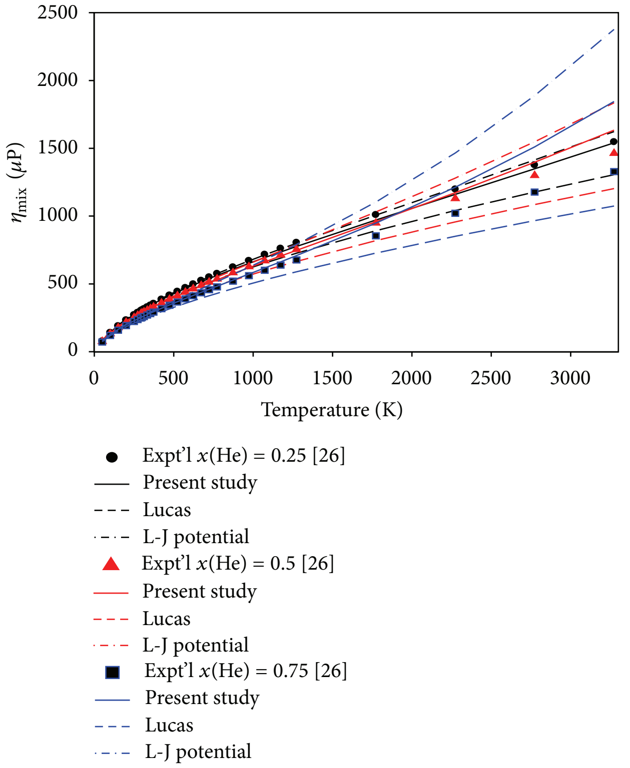

Figure 22: Comparison of measured and calculated viscosities for He + Ne mixture.

Kihara potential with group contribution concept, and the Tsonopoulos correlations. For the viscosity calculations, the proposed model agrees better with the observed and calculated data than the original Lennard-Jones (12-6) potential, the Kihara potential with group contribution method, the Lucas method, the Simsci Database, and the Refprop Database. Agreement between experimental and calculated thermal conductivities obtained by the proposed model

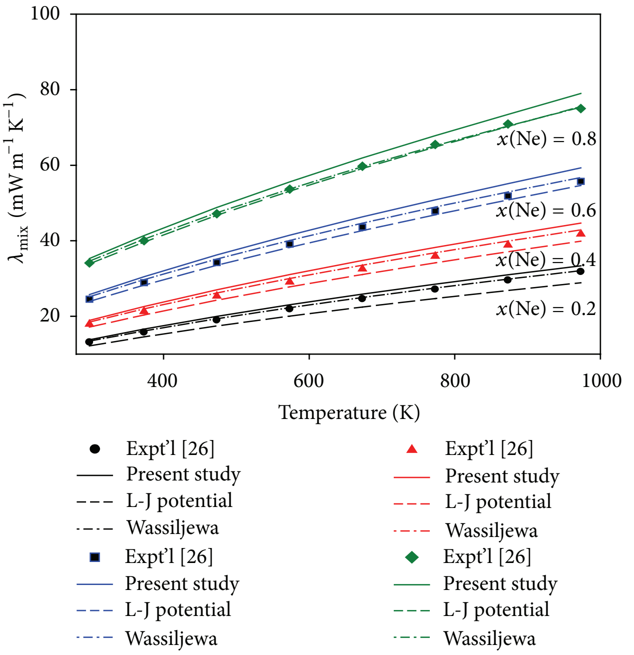

FIGURE 23: Comparison of measured and calculated thermal conductivities for Ne + Kr mixture.

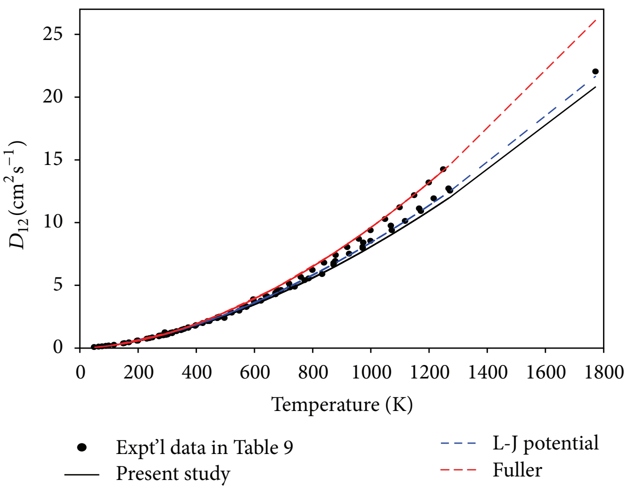

FIGURE 24: Comparison of measured and calculated binary diffusion coefficients for He + Ne mixture.

is somewhat less accurate than the Simsci Database, but compares very well with the original Lennard-Jones (12-6) potential and with the Refprop Database. Calculation of self-diffusion coefficients shows that this work is in better agreement with experimental data than those of the original Lennard-Jones (12-6) potential and of the Fuller method, and that for helium gas and for neon gas results of the proposed method is less accurate than the original Lennard-Jones (12-6) potential.

For mixture property predictions, the same set of potential parameters is applied with no additional parameters. Second cross-virial coefficient data calculated by the present study is less feasible to those of Dymond's correlations and is in better agreement with the observed data than the original Lennard-Jones (12-6) potential and the corresponding states method of Tsonopoulos. The present study is in better agreement between experimental mixture viscosity data than the original Lennard-Jones (12-6) potential and the Lucas method, except for the mixture of kr + Xe. The present study is in somewhat worse agreement between measured and calculated mixture thermal conductivities than the Wassiljewa equation with the combinational factor of Mason and Saxena and is more accurate than the original Lennard-Jones (12-6) potential. However, thermal conductivity of the He + Ne and Kr + Xe mixtures was reproduced better with the Wassiljewa equation than with the proposed method. The present study is in appreciably better agreement between the observed and calculated binary diffusion coefficients of noble gases mixtures than the original Lennard-Jones (12-6) potential and the Fuller method.

In this work, the empirical approach of adding a temperature-correction parameter to the reduced temperature in the Lennard-Jones (12-6) potential function has been tested with good success for the calculations of thermodynamic and transport property of noble gases and their binary mixtures in dilute gas region. Application of this approach to other substances such as polyatomic, polar gases will be tested in the near future.

Nomenclature

A:	Combinational factor in (18)
A^*:	Defined by (13), $\Omega^{(2,2)*}(T^*)/\Omega^{(1,1)*}(T^*)$
B:	Second virial coefficient (cm^3 mol^{-1})
D:	Diffusion coefficient (cm^2 sec^{-1})
k_B:	Boltzmann constant, $1.3806488{\cdot}10^{-23}$(JK^{-1})
M:	Molecular weight (gram mol^{-1})
N_A:	Avogadro constant, $6.022{\cdot}10^{23}$(mol^{-1})
P:	Pressure (bar)
R:	Distance between molecular centers of molecules 1 and 2 (Å)
RMSD$_r$:	Root-mean-square deviation (cm^3 mol^{-1})
%RMSD$_r$:	Percent relative root-mean-square deviation, relative (%)
T:	Absolute temperature (K)
T^*:	Reduced temperature, $k_B(T-\tau)/\varepsilon$
U:	Intermolecular potential function
y:	Mole fraction in the gas phase
X_η:	Defined by (10)
Y_η:	Defined by (11)
Z_η:	Defined by (12).

Greek Letters

ε:	Depth of the potential well [J]
η:	Viscosity (μP)
λ:	Thermal conductivity (mW m^{-1} K^{-1})
σ:	Collision diameter (Å)
τ:	Reduced temperature-correction parameter

$\Omega^{(1,1)*}$: Collision integral for diffusion coefficient
$\Omega^{(2,2)*}$: Collision integral for viscosity.

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